

# Recoil effects in the hyperfine structure of QED bound states

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The authors give a general discussion of the derivation from field theory of a formalism for the perturbative solution of the relativistic two-body problem. The lowest-order expression for the four-point function is given in terms of a two-particle three-dimensional propagator in a static potential. It is obtained by fixing the loop energy in the four-dimensional formalism at a point which is independent of the loop momentum and is symmetric in the two particle variables. This method avoids awkward positive- and negative-energy projectors, with their attendant energy square roots, and allows one to recover the Dirac equation straightforwardly in the nonrecoil limit. The perturbations appear as a variety of four-dimensional kernels which are rearranged and regrouped into convenient sets. In particular, they are transformed from the Coulomb to the Feynman gauge, which greatly simplifies the expressions that must be evaluated. Although the approach is particularly convenient for the precision analysis of QED bound states, it is not limited to such applications. The authors use it to give the first unified treatment of all presently known recoil corrections to the muonium hyperfine structure and also to verify the corresponding contributions through order  $\alpha^2 \ln \alpha E_F$  in positronium. The required integrals are evaluated analytically.

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## I. INTRODUCTION

### A. History and background

The study of hydrogenlike systems has played a major role in the development of modern physics, from the original understanding of the spectra in terms of quantum mechanics, through such refinements as relativistic, spin-orbit, and quantum electrodynamic (QED) contributions, to the present concern with precision tests of relativistic two-body theory in such diverse systems as hydrogen, positronium, muonium, and quarkonium. The "modern" era dates from the late 1940s, when experimental discoveries stimulated the evolution of quantum electrodynamics to its present precise form. This era has been one of interplay between experiment and theory, in which each has encouraged increasing refinement in the other. On the experimental side, this evolution has led to the development of very sophisticated techniques, while on the theoretical side it has required the development of more and more powerful methods of calculation. Over the years, theory and experiment have been in agreement more often than in disagreement. Although there have been occasions when there seemed to be real conflicts between them, new experiments or better calculations ultimately led to resolution. At the present time there seem to be no such conflicts, but there are situations in which it is feasible to improve theory and experiment to provide more stringent tests of our basic theory. Once again, it appears that progress on the theoretical side requires the development of more sophisticated methods. It is such methods that are the topic of this paper.

High-precision bound-state calculations are different in character from other precision calculations, such as the electron anomaly. The latter requires the highest refinement in perturbative analysis in renormalization, including intricate subtractions of overlapping and nested divergences. Renormalization theory in QED is a perfectly well-defined procedure in terms of an expansion in numbers of photons, but its implementation is tedious. To give an indication of the magnitude of this effort, we may note that the four-photon contribution theory, which is the present scene of action (Kinoshita and Lindquist, 1981), involves the analysis of 891 graphs, a small fraction of which can be done analytically. The algebraic analysis of these graphs, as well as the subsequent integrals, is accomplished with the aid of large computers. Each integrand is composed of 5000 to 15000 terms and some have ten variables of integration. On the other hand, precision bound-state calculations are essentially nonperturbative. Though they involve kernels which can be written in terms of Feynman graphs, the dimensionless parameters, particularly the fine-structure constant  $\alpha$ , enter the wave functions and the particle propagators (through the energy) in a nonperturbative way. Thus one cannot simply count powers of  $\alpha$  in a given kernel in order to determine its ultimate contribution to an energy shift. As a consequence, the formal development of bound-state theory is not at all mechanical. There are

many routes to a correct answer, and they are not equally felicitous. Fortunately, the tedium involved in exploring various of these paths is partially offset by the fact that the ultimate work involved in algebra and integrals is orders of magnitude simpler than that of the electron anomaly—provided the formal analysis is well chosen.

In spite of the statement in the preceding paragraph that bound-state theory is nonperturbative, it is possible to make use of small parameters such as  $\alpha$  and  $m_e/m_A$  (where  $m_A$  is the mass of the nucleus) to develop expressions in increasing orders of smallness. However, the nonperturbative nature of the expansion shows up in nonanalytic dependence on these parameters (such as logarithms). As indicated in the preceding paragraph, there is an art in developing a theoretical expression in this manner. At the most elementary level, one must be aware that there are nonanalytic terms and seek them out; the trick is to arrange the remainder in a tractable form so that its analytic part of the same order is easily extracted and terms of higher order isolated. Usually it is best to do this before integrations are carried out, rather than later. We can then make an estimate of the accuracy of our calculation by guessing the size of neglected terms, which have additional factors of the small parameters. Such estimates can be very unreliable; one should be aware of the danger of putting them on the same level as experimental errors.

In the precision study of hydrogenlike bound-state energy levels, there are three main categories of effects to be considered. The first category consists of *radiative corrections*, a term referring to corrections due to the emission and absorption of photons by the electron and also to vacuum polarization corrections to the exchanged photon propagators. In these, the recoil of the nucleus is ignored except for the dependence of quantities on the reduced mass rather than  $m_e$ . The treatment of renormalization is similar to that for free electrons, except that electron propagators in an external Coulomb field are used [Furry (1951) representation]. The second category consists of *recoil corrections*, in which more dynamical effects due to nuclear recoil are incorporated; here radiative corrections are ignored, except to the extent that it may be legitimate to include a particle's anomalous moment. Until recently, it was quite possible to keep these two categories separate to the order of interest. Thus it was possible for a worker to be an expert on radiative correction effects without understanding the complications of recoil, and vice versa. Now, the level of accuracy has reached the point where both complications must be treated together as *radiative-recoil* corrections. However, in combination some of the subtleties of each category are absent. (At some level it is necessary to include a fourth category consisting of other small effects such as weak interactions, finite nuclear size, nuclear polarizability, etc.)

In this paper, we are concerned principally with recoil effects—that is, with corrections associated with the small parameter  $m_e/m_A$ . However, it would be unwise to attempt to expand in this parameter directly (aside from the nonanalytic dependence which would be encountered), be-

cause the leading effects can be incorporated in the use of the reduced mass [ $m_r \equiv m_e m_A / (m_e + m_A)$ ]. It would immensely complicate the analysis to expand in powers of  $m_e/m_A$  instead. There is probably no precise definition of the separation between reduced mass and intrinsic recoil effects beyond the leading order terms, but we try to keep the mass symmetry as long as possible. Thus a portion of the results, which can be characterized in terms of its  $\alpha$  dependence, is valid for the equal mass case (positronium).

Every physicist knows the trivial analysis for separating the center of mass and relative motion in the nonrelativistic two-body system to find a simplified problem in which the relative motion is described using the reduced mass. When one or both particles are to be treated relativistically, there is no similar simple procedure. In fact, if one starts with a two-body system and lets one of the particle masses become infinite, it requires a nontrivial analysis to demonstrate that the result can be expressed in terms of a relativistic equation for the other particle in a central potential. The physics is clear; it is simply the formalism which is awkward. We now trace briefly the history of the development of our understanding of the recoil problem. Since this paper is also concerned with the particular example of the hyperfine splitting, we also review its development briefly. It is not our aim to present a complete or critical survey of the literature. Rather it is to give a general perspective of the subject.

## 1. Early work

The first main step in treating the recoil problem involving Dirac particles was due to Breit (1929). In that work he presented his famous equation for two electrons interacting through the electromagnetic field. That equation has the form of an instantaneous interaction between the electrons, but it does incorporate retardation effects to the extent that they are important at the  $v^2/c^2$  level. He was guided by the classical result but arrived at the equation by a somewhat laborious analysis. His equation was the only one used for the treatment of recoil effects for over two decades. In fact, there were very few workers in the field, other than Breit and his associates, during that period. It took the stimulation of subsequent experiments to bring on the development of more precise formulations.

The first formulation of the theory of hyperfine splitting (hfs) was due to Fermi (1930). Traditionally the leading contribution to the ground-state hfs is referred to as the "Fermi splitting":

$$E_F \equiv \frac{8}{3} \alpha^4 c^2 \frac{m_r^3}{m_e m_A} = \frac{16}{3} \alpha^2 \left[ hc R_\infty \frac{m_r}{m_e} \right] \frac{m_r^2}{m_e m_A}, \quad (1.1)$$

where  $m_r$  is the reduced mass,  $m_e$  the electron mass,  $m_A$  is the mass of the nucleus, and  $R_\infty (=m_e c \alpha^2 / 2h)$  is the

Rydberg for infinite nuclear mass.<sup>1</sup> To obtain his result, Fermi used the Dirac equation but made an approximate two-component reduction. Breit (1930) treated the Dirac wave functions without approximation and derived a correction factor to (1.1), which we refer to as the Breit relativistic correction; for the ground state, this factor takes the form  $(1 + \frac{3}{2} \alpha^2 + \dots)$ . The correct reduced mass factor was not supplied at that time, perhaps because of the complications of dealing properly with recoil for the Dirac equation. In any case, experimental precision at the time did not require such refinements.

The theoretical situation was improved by Breit and Meyerott (1947), who used the Breit equation to find the correct reduced-mass dependence. They were stimulated by the experimental work of Nafe, Nelson, and Rabi (1947). Breit and Meyerott also predicted corrections of relative order  $\alpha^2(m_e/m_A) \ln \alpha$ , but not the much larger terms of relative order  $\alpha(m_e/m_A) \ln(m_A/m_e)$ . The latter terms require treatment of two-photon kernels. Stimulated by the experiment of Lamb and Retherford (1947), Breit and Brown (1948) analyzed the effect of nuclear motion on the fine structure of hydrogen. Their work refers to recoil, but not radiative corrections. The object was to see whether recoil effects remove the Dirac degeneracy. They demonstrated that the recoil terms of order  $\alpha^2(m_e/m_A) R_\infty$ —which could potentially have given a very large contribution—cancel. In their work this cancellation appears as an almost fortuitous compensation between various expectation values involving Dirac wave functions. In our work, this effect shows up as a compensation between a contribution arising from pure Coulomb interactions and one arising from the convection part of the nuclear current. Further progress in the use of the Breit equation was made by Breit, Brown, and Arfken (1949); but they noted its limitations in a concluding remark (see p. 1304), "A complete treatment of the problem requires a more consistent application of electrodynamics than that given here." Breit, Brown, and Arfken also estimated the order of magnitude of the finite-size correction for the proton structure, using a rather crude model for the (at that time unknown) current distribution of the proton. In an associated paper, Brown and Arfken (1949) discussed the effect of proton radius on the nuclear motion correction.

## 2. Radiative corrections

As experiments became increasingly accurate, theory became more refined. Rather than review these developments chronologically, we discuss first the "radiative corrections," which can be understood without recourse to

<sup>1</sup>This expression is based on Dirac magnetic moments for both particles. Sometimes the Fermi splitting is expressed in terms of the total magnetic moment of the nucleus. We avoid this here because some of the terms in our analysis are not proportional to the total magnetic moment. The reader should be warned in comparing results from different papers to take into account these different conventions.

a complete relativistic two-body formalism. The main effect of the radiative corrections is to supply the electron with an anomalous magnetic moment, which can be incorporated into the hfs simply by multiplying the Fermi splitting by the factor  $(1 + a_e)$ . In the context of the hfs, the term *radiative corrections* is usually used to refer to the additional effects due to the binding. (Sometimes this is indicated in formulas by using  $Z\alpha$  as the expansion parameter associated with binding.) Only one-photon radiative corrections (with all orders of the Coulomb interaction) have been considered so far, and the work required to attain the present level of accuracy has extended over three decades.

The first improvement in the theory of the hfs (beyond incorporating the electron's anomalous magnetic moment) was the calculation of contributions to order  $\alpha^2 E_F$  by Kroll and Pollock (1951,1952) and Karplus, Klein, and Schwinger (1951). The terms considered were those involving the electron self-energy and the vacuum polarization. Because some contributions arise from very small atomic momenta, a nonperturbative treatment of the Coulomb interaction was essential. (This is also a feature of the Lamb-shift calculation.)

The next step was to improve the calculation of corrections from the same graphs to order  $\alpha^3(\ln^2\alpha$  or  $\ln\alpha)E_F$ . This was accomplished by Layzer (1961,1964) and Zwanziger (1961,1964). Because they were seeking "nonanalytic terms," they could use the free-propagator expansion for the electron propagator in a background Coulomb field. This work was verified by Brodsky and Erickson (1966), who used a gauge-invariant reduction for the electron self-energy in the presence of an external field. The latter method had been previously applied to the Lamb shift by Erickson and Yennie (1965a,1965b). Brodsky and Erickson also estimated the term of order  $\alpha^3 E_F$ . The latter term has recently been calculated numerically by Sapirstein (1983) to the level of accuracy currently needed.

The radiative corrections just described produce additional terms in the factor multiplying the Fermi splitting—i.e., they are to be added to the Breit relativistic correction and the anomalous moment term  $a_e$ . This is because the characteristic momentum in these contributions is very small compared to that in the contribution giving the basic Fermi splitting. In addition, all these corrections are to be multiplied by the ratio of the total magnetic moment of the nucleus to its Dirac value. This is because for these contributions the nucleus is serving as a static source of electric and magnetic fields. However, for positronium more care is required, because the characteristic momentum in the nuclear anomalous magnetic moment contributions is then of the same order as that in the radiative correction contributions.

### 3. Recoil corrections

We turn now to a description of the development of the "recoil corrections." The calculation of such corrections is obviously related to the development of the theory of a relativistic two-body system. There is a vast amount of

literature concerning this theory. Much of it is directed toward applications other than hfs, some of it is purely formal and does not address any particular bound-state problem, and some of it is relevant to the treatment of the energy shifts of interest here. We shall mention only the highlights of this development except for work which seems to be similar to our own. We wish to warn the reader that we are not attempting to give a complete or balanced presentation.

During the 1950s, most of the activity involved the Lamb shift and hyperfine splitting in hydrogenic systems. Because the only systems experimentally accessible for many years were hydrogen and positronium, most of the effort concentrated on them. Many of the results for hydrogen are directly transferable to muonium, of course, with a simple change of the mass and magnetic moment of the nucleus. However, as anticipated by Breit and his collaborators, certain of the hydrogen results are sensitive to the finite internal size of the proton. Even if one is not considering the effects of recoil, the finite size of the proton enters the expression for the hfs. Obviously, a softening of the interaction at small distances reduces the hfs. The effect was first analyzed completely by Zemach (1956), who took into account the combined effect of charge and current distribution and found a correction of order 40 ppm—which is actually more important than the recoil corrections. Closely related to the spatial structure of the proton is the more general issue of internal dynamics, which ultimately limits our ability to use the present very accurate value of the hydrogen hfs as a test of our theories. At the present level of understanding, one attempts to account for the dynamical effects with "proton polarizability corrections." The development of a systematic method of accounting for these effects, based purely on theory or on independent experimental measurements, is one of the important unsolved problems in the field.

The earliest treatments of the relativistic two-body system made use of the Breit equation. The Breit equation does not produce corrections of relative order  $am_e/m_A$  in the fine structure or hyperfine structure. As was pointed out by Salpeter (1952), the reason is that it corresponds essentially to a single-electron theory, rather than to hole theory. Thus these contributions, which are present and experimentally relevant, can be found only if the equivalent of hole theory is used. As experimental precision increased,<sup>2</sup> it became necessary to develop a more accurate formalism based on a complete field theoretic treatment of the two-body problem. This was done by Schwinger (1951) and by Salpeter and Bethe (1951). The result is now usually referred to as the Bethe-Salpeter equation. It is now generally recognized that this equation, which is a homogeneous four-dimensional integral

<sup>2</sup>The experimental history of the hydrogen hyperfine structure will not be reviewed here. Presently, the splitting in the ground state is known to better than one part in  $10^{12}$  (Hellwig *et al.*, 1970; Essen *et al.*, 1971). In contrast, current theory has an accuracy of order 1 ppm.

equation, is not in a practical form for high-precision analysis of energy levels. The first systematic approximation procedure for solving this equation was developed by Salpeter (1952), who showed how to develop a perturbation expansion in which the starting point is a solvable three-dimensional equation. Present work is also generally based on some three-dimensional formulation which incorporates varying amounts of the basic physics. Additional field-theoretic effects are incorporated through various perturbation kernels. There is considerable freedom of choice in dividing the problem into a zeroth-order part and a perturbation part; but all methods should yield equivalent results.

Salpeter's (1952) original formulation of a three-dimensional approach was directed toward the Lamb-shift problem, where he found a contribution of relative order  $m_e/m_p$ . (Note that there are no additional powers of  $\alpha$  compared to the leading effect.) Salpeter also noted the existence of the leading recoil corrections to the hfs. Using Salpeter's three-dimensional approach, Karplus and Klein (1952) studied the hfs in the positronium system. They found a term of the same order as the Fermi splitting which arises from the simplest annihilation graph, and also a correction of order  $\alpha E_F$ . Karplus and Klein found it necessary to introduce a temporary infrared cutoff in order to control the spurious divergences that arise from neglecting the binding energy in parts of their calculation. These results were confirmed by Fulton and Martin (1954), who used the Salpeter equation, but avoided the cutoff by using more accurate expressions for the fermion propagators. In the case of the hydrogen hfs, Arnowitt (1953) and Newcomb and Salpeter (1955) calculated the leading recoil corrections. One can use Arnowitt's intermediate results to find the mass-symmetric contribution for the part independent of the anomalous magnetic moment of the proton. They found that, with regard to its anomalous magnetic moment, the proton could not be treated as pointlike without introducing divergences. Thus it was necessary to take the finite size of the proton into account in an intrinsic way; however, they found that there is only a logarithmic dependence on this size. Aside from this complication, these corrections are of order  $\alpha(m_e/m_p)E_F$  in the hydrogen hfs. Much later, these results were confirmed by Grotch and Yennie (1967,1969), who used an effective-potential formalism designed to reproduce the field-theoretic scattering amplitudes to sufficient accuracy.

From now on, we restrict our attention to muonium<sup>3</sup> and positronium<sup>4</sup> hfs. Certain parts of the theoretical analysis for hydrogen can be applied directly to muonium, but other parts are no longer valid, since the muon should

be treated as an elementary particle rather than a composite one. Contributions which arise from the low-momentum region (i.e., low enough to be insensitive to the nucleon size) can generally be taken over for muonium. The anomalous moment part of the radiative corrections to the muon can be accounted for by inserting a factor  $(1+a_\mu)$  in the expression for the Fermi splitting (1.1). The reason is that the momenta which are relevant for that leading term are at most of the order of the electron mass, so that the form factor associated with the muon's anomalous moment is irrelevant. This remark applies also to the Breit relativistic correction, as well as to the radiative corrections to the electron and exchanged photon lines. However, the muon's anomalous moment does not multiply the recoil corrections which have been calculated. If the recoil contribution in hydrogen is examined in the limit in which the proton size is neglected, it is found that there is no term which is linear in the anomalous moment. (The term *quadratic* in the anomalous moment diverges as the proton size shrinks to zero; the implication of this for muonium is that the two-photon radiative correction for the muon line cannot be expressed in terms of the anomalous moment. In any case, the two-photon radiative correction contribution is estimated to be a couple of orders of magnitude smaller than terms of current interest.) Note that the recoil contribution is perfectly symmetric in the masses of the two particles so that it is valid for positronium in the limit in which the masses become equal.

The order of magnitude of the leading recoil corrections for the muonium hfs is  $\alpha(m_e/m_\mu)\ln(m_\mu/m_e)E_F$ ; the corresponding contribution in positronium is of order  $\alpha E_F$ . In the muonium case, the  $\ln(m_\mu/m_e)$  dependence indicates that this contribution arises primarily from momenta between  $m_e$  and  $m_\mu$ . The correct mass-symmetric treatment of it (Arnowitt, 1953) requires that both the electron and the muon be treated relativistically to this order in  $\alpha$ . In order to make a comparison with precision experiments, it is necessary to calculate the recoil corrections to higher order in  $\alpha$ . It turns out that the dominant part of these contributions arises from the low-momentum region ( $\alpha m_r \leq p \leq m_e$ ) and has the orders  $\alpha^2 \ln \alpha E_F$  for the positronium hfs and  $\alpha^2(m_e/m_\mu) \ln \alpha E_F$  for the muonium hfs. In the calculation of these contributions, it turned out that Salpeter's original method was very awkward, as it led to a proliferation of terms. Thus the original work on these contributions was carried out in piecemeal fashion. Fulton, Owen, and Repko (1971a,1971b), who first discovered the existence of the  $\ln \alpha$  terms, used a Salpeter-equation approach to do a calculation of the contribution due to the exchange of at least one transverse virtual photon. Barbieri and Remiddi (1976) developed a perturbation approach based on the Salpeter equation, which they used to calculate some contributions due to exchange of three photons in muonium and positronium and also some annihilation contributions in positronium. Cung, Fulton, Repko, and Schnitzler (1976) made a tensor decomposition of the Salpeter equation in order to obtain an effective Hamiltonian, and then

<sup>3</sup>While we do not review the experimental studies of muonium, we note that it was discovered by Hughes *et al.* (1960) and that its detection depended on the fact that the  $\mu^+$  forming the bound state with an electron was produced initially in a parity-violating decay. For a review, see Hughes and Kinoshita (1977).

<sup>4</sup>Positronium was discovered experimentally by Deutsch (1951); a recent review was given by Rich (1981).

used the Hamiltonian to calculate a contribution to the positronium hfs due to exchange of three Coulomb photons.

The first unified treatment of the terms of order  $\alpha^2 \ln \alpha E_F$  for positronium and  $\alpha^2 (m_e/m_\mu) \ln \alpha E_F$  for muonium was given by Lepage (1977). He developed a perturbation expansion for the Bethe-Salpeter equation by choosing a zeroth-order kernel which fixed the time component of momentum, so that one particle is on the mass shell. The resulting integral equation, which is similar to one suggested by Gross (1969), has the form of the Coulomb-Dirac equation. Lepage's result for the one-transverse-photon contribution to the hfs differs from that of Fulton, Owen, and Repko (1971a, 1971b). This disagreement was resolved in favor of Lepage by Bodwin and Yennie (1978), who gave a complete treatment of exchange-photon contributions to the above order using a refined treatment based on the Salpeter equation.

Caswell and Lepage (1979) first computed the order  $\alpha^2 \ln \alpha E_F$  contributions to the positronium hfs that arise from two-photon annihilation kernels. Cung, Fulton, Devoto, and Repko (1977, 1978a) gave the first complete calculation of the order  $\alpha^2 E_F$  contribution to the positronium hfs due to three-photon annihilation kernels. They also computed the contribution in this order that comes from the virtual annihilation of two photons accompanied by radiative corrections [Cung, Devoto, Fulton, and Repko (1978b)].

In obtaining the  $\ln \alpha$  contributions, it was necessary to use nonrelativistic approximations for both the electron and the muon, after the relativistic terms of lower order had been removed from the analysis. Then the final integrals were cut off at the electron mass. It was realized that the relativistic electron region might produce contributions containing  $\ln(m_\mu/m_e)$  in the same order of  $\alpha$ . This possibility was investigated by Bodwin, Yennie, and Gregorio (1978). Since their method of analysis based on the Salpeter equation had become completely intractable for these terms, they used a Gross equation similar to that of Lepage. They found that all terms of order  $\alpha^2 (m_e/m_\mu) \ln(m_\mu/m_e) E_F$  due to exchanged photons cancel. Caswell and Lepage (1978b) gave a simple argument for this cancellation based on the symmetry of the integrands.

Caswell and Lepage (1978a) and Barbieri and Remiddi (1978) independently developed a formalism in which the lowest-order problem is expressed in terms of the Coulomb-Schrödinger one. Caswell and Lepage used it to obtain "sum over states" terms of order  $\alpha^2 (m_e/m_\mu) E_F$  for muonium hfs and  $\alpha^2 E_F$  for positronium hfs. Their result was confirmed by Buchmüller and Remiddi (1980). Bodwin, Yennie, and Gregorio (1982) used an improved three-dimensional formalism to complete the calculation of terms of order  $\alpha^2 (m_e/m_\mu) E_F$ . The present paper describes this method in detail.

#### 4. Radiative-recoil corrections

It was pointed out by Caswell and Lepage (1978b) that, in addition to the contribution to the hfs due purely to

photon exchange, there are "radiative-recoil" contributions which are important at the present level of accuracy. This brings the previously separate lines of investigation together. These contributions arise from photon exchange accompanied by radiative corrections to the fermion legs or to the photon propagator. Caswell and Lepage calculated the term of order  $\alpha^2 (m_e/m_\mu) \ln^2(m_\mu/m_e) E_F$  in muonium, using their Coulomb-Schrödinger formalism. The terms of order  $\alpha^2 (m_e/m_\mu) \ln(m_\mu/m_e) E_F$  in muonium were calculated by Terray and Yennie (1982) and the terms of order  $\alpha^2 (m_e/m_\mu) E_F$  in muonium and  $\alpha^2 E_F$  in positronium by Sapirstein, Terray, and Yennie (1983, 1984). Their reduction of the energy shifts makes use of fairly sophisticated procedures, some of which we describe later.

#### 5. Other three-dimensional wave equations

As mentioned before, modern precision calculations of bound-state energies are based on three-dimensional formulations of the basic wave equation, with corrections inserted as perturbation kernels of various sorts. We indicate here some of the highlights of the development of these formulations without attempting to be complete.<sup>5</sup> Some of these are described in more detail in the following section. As emphasized by Lepage (1977), an arbitrariness in the choice of a three-dimensional formalism arises from the fact that there is no unique choice for the free propagator which occurs in the zeroth-order integral equation. Different choices of propagator simply lead to different perturbation kernels. Thus there is freedom to choose the initial approximation in any convenient way for the particular problem under consideration. A well-known approach was developed by Blankenbecler and Sugar (1966), but their effort was directed more at the multichannel scattering problem. Many of these approaches contained an awkward feature that relativistic energies involving square roots occurred in the denominator of the propagator. This makes it difficult to find closed-form analytic solutions as the starting point of a perturbation treatment and leads to intractable integrals in low orders of perturbation theory. Using certain assumptions (on-shell unitarity and the linearity of the inverse propagator in  $\mathbf{p}^2$ ), Todorov (1971) arrived at an equation, which has many features in common with ours. Austen and de Swart (1983) give a field-theoretic derivation of an

<sup>5</sup>In addition to the original work of Salpeter (1952) and other papers previously mentioned, a sampling of other papers dealing with three-dimensional relativistic equations is Levy (1952a, 1952b), Klein (1952, 1954), Macke (1953a, 1953b), Logunov and Tavkhelidze (1963), Blankenbecler and Sugar (1966), Grotch and Yennie (1967, 1969), Gross (1969), Kadyshevsky (1968), Itzykson *et al.* (1970), Todorov, (1971), Yaes (1971), Faustov (1972), Klein and Lee (1974), and Gorelick and Grotch (1977).

equation—which is also similar to ours—in which the potential takes into account an important part of the physics of planar and crossed two-photon exchanges. In all of these three-dimensional formalisms, the loop energy  $p_0$  is fixed by some procedure; and the difference between the full kernel and the fixed one is treated with the other perturbations. There is freedom of choice both on the value at which  $p_0$  is fixed and the terms which are kept in the residue of the product of the two particle propagators.

Our particular procedure retains the mass symmetry in the choice of the point at which  $p_0$  is fixed, but introduces mass asymmetry in the residue by retaining the full Dirac numerator structure for the lighter particle but not for the heavy one. Thus we have some of the dynamics necessary for obtaining mass-symmetric results. Our method works best when there is a large mass ratio, but it has utility for positronium as well. In this paper, we apply it to a detailed calculation of contributions to hfs arising from exchange photons. We recover, in a unified treatment, all previously known contributions of this type for muonium and positronium and also give a detailed account of the recent calculation of the order  $\alpha^2(m_e/m_\mu)E_F$  nonlogarithmic terms in muonium.

## B. Description and organization of the present calculation

Although our formalism is similar to many others existing in the literature, in order to avoid any confusion or ambiguity we start in Sec. II with a derivation of our perturbation scheme from first principles. In proceeding to the refined orders of magnitude of interest in the hyperfine splitting (hfs) and in other bound-state calculations (usually of relative order  $10^{-6}$ , corresponding to  $\alpha^3$  or  $\alpha^2 m_e/m_\mu$ ), great precision in all details is essential. We find terms of the order of interest arising from many different, apparently unrelated, places in the calculation.

The organization of the analysis presented in this paper was arrived at after much trial and error. In earlier versions, it was plagued by spurious terms which compensated in a seemingly miraculous way. In some cases these terms were even divergent before the compensation. We have managed to arrange the analysis to eliminate many of them from the beginning, but probably even greater simplifications are possible. It is difficult for us to state a general principle which would have led us more directly to a viable approach. However, there are some minor principles which provide useful guidance in avoiding certain difficulties. Very likely, if one wishes to go to higher orders than contemplated here, further refinements in the approach would be necessary. Our expectation is that some combination of analytic work to extract the first few orders would have to be combined with a somewhat sophisticated numerical analysis to get results of a few factors of ten better than is presently required.

One of our goals in this work is to extract all previously calculated contributions in a systematic way. To our knowledge, this has not been done before, even though

workers in the field have satisfied themselves about the consistency of the earlier calculations. The difficulty has been that for different contributions different approximation procedures are appropriate. When extracting “non-analytic” terms, it is not difficult to make such approximations consistently, since different kinematic regimes and different analytic structures are easy to identify and isolate. The present complication is that we are seeking analytic terms which are small residues of the earlier terms. The only safe approach is to use a unified approximation scheme—certainly this was revealed over and over again during the course of the present work.

Although we hope that it will be possible for the dedicated reader to reconstruct as much of the calculation as desired, we have tried to organize the presentation so that it is possible to follow the discussion at different levels. In the remainder of the Introduction, we try to provide guidance for those who wish primarily to study the main features of the analysis.

Section II is concerned with obtaining a workable perturbation formalism for analyzing the energy shifts. For this purpose we are not interested in the details of the (Bethe-Salpeter) wave functions, which can be quite complicated. However, from time to time we point out structures which may be incorporated into the wave function. Although our approach is based on the Bethe-Salpeter philosophy, the practical procedure is rather different. To solve the Bethe-Salpeter bound-state integral equation directly to the required accuracy seems to us to be quite awkward and not at all useful. A well-known complication is that it is difficult to obtain the correct result in the limit in which the mass of one of the particles becomes infinite. The correct treatment of that limit requires the use of kernels with crossed photon lines of arbitrarily high order.<sup>6</sup> In the present and in most other recent approaches, the calculation is arranged differently, so that this problem does not occur.

Our procedure is to analyze the positions of the poles in the total energy in the four-point function (two particles in and two particles out). The perturbation approach works because in QED the two-particle component of the state dominates the wave function. The first step is to simplify the four-point function to one which is exactly calculable and whose bound-state poles are close to the correct one. This is done by first considering only ladder graphs with Coulomb rungs, since the Coulomb interaction dominates the binding. This is very natural in the Coulomb gauge, of course; but we may also use the Coulomb potential as an initial approximation in a covariant gauge. In the latter case, Lepage (1980) has shown us how to arrange the calculation so as to avoid the difficulties encountered by Love (1978). We believe that our methods are not restricted to QED. They might, for example, provide a more fundamental approach to quark-pair bound-state theory in which one starts with an effective

<sup>6</sup>A demonstration of this fact is given by Brodsky (1969) and Gross (1982).



tive potential and then corrects it by a perturbation expansion. The choice of the starting potential for a particular application represents a compromise between a desire to simplify the lowest-order equation and a desire to minimize the contribution of perturbations.

Since it seems to make the exposition simpler, in the present work we use the Coulomb gauge. However, after the perturbation expansion is developed, in Sec. III.B we rearrange the kernels so that they can be treated in the Feynman gauge. This has the advantage of eliminating awkward noncovariant denominators as well as the more complicated algebraic structure of the transverse photons.

Returning to the discussion of the Coulomb ladder graphs, we reduce the four-dimensional loop integrals to three-dimensional ones by fixing the energy component in some manner. There are various options available in carrying out this step. All of them lead, with suitable approximations, to the nonrelativistic Schrödinger equation. The original approach of Salpeter (1952) was simply to carry out the integration over the loop energy, using the fact that the Coulomb propagators are independent of that variable. However, this leads to expressions which are exceedingly difficult to use in the very refined calculations now being carried out: they have positive and negative (plane-wave) projection operators for each particle, but even worse, they involve the relativistic energies of the particles [in the form  $(\mathbf{p}^2 + m^2)^{1/2}$ ]. This appears to make analytic work of higher order hopeless in this approach. As alluded to earlier, the infinite-mass limit does not appear automatically in this approach. Rather, it must be fixed up in each order in  $\alpha$  by incorporating the effects of crossed graphs.

Another approach, which we actually used during the trial-and-error era of this work, is to extract a contribution in which the heavier particle is put on the mass shell. The resulting equation is known as the Gross (1969) equation. This also leads to expressions involving the relativistic energy of the heavier particle, but the denominator containing this square root can be rationalized and the numerator can be rearranged so that the dominant terms do not involve the square root. The method seems quite promising. However, there are contributions in which the square roots are awkward. For example, they occur in photon denominators in such a way that they appear almost negligible; but in fact they cause separate integrals to diverge, and it is necessary to group various contributions together very carefully in order to avoid these spurious problems.

Our final approach is to fix the loop energy in a way which is independent of the three momentum (in the center-of-mass frame). Our experience so far is that this works very well for calculating the recoil terms to the hfs; but it may not work as well in the recoil corrections to the leading radiative correction term in the Lamb shift. Using this approach, we find the leading contribution takes the form of the Dirac equation for the electron, with a large-component projector for the muon. The strength of the Coulomb interaction is modified slightly by a reduced mass factor; this modification leads to the correct

reduced mass effects in the nonrelativistic regime. Actually, we find it advantageous to modify the interaction potential slightly, replacing the Coulomb interaction with the form found by Grotch and Yennie (1967,1969). This is a practical technical point of no fundamental significance; it allows us to eliminate certain cancelling contributions early in the calculation.

The previously described treatment is presented in Sec. II.A.1. It yields an approximate four-point function, which may be expressed as a sum over Dirac-Coulomb wave functions. In Sec. II.A.2, we develop a systematic perturbation theory for evaluating higher-order terms. We have to correct for the approximation to the Coulomb ladder and for kernels containing crossed Coulomb photons and ones containing transverse photons. The resulting set of perturbation kernels is not unique. Depending on the choice of perturbation expansion, a given contribution can show up in various kernels and in various orders of perturbation theory. In order to simplify the calculation, we have formulated the perturbation expansion in a particular way, which probably will not appear to the reader to be the most direct. We hope that the merits of our choice will become apparent as the calculation itself is scrutinized.

In Sec. II.B we describe the leading spin-independent kernels. It is found that the nonrecoil residue from the Coulomb ladder nicely compensates the nonrecoil contribution from the simplest crossed Coulomb line. This type of compensation continues to work for more complicated Coulomb graphs—a result long known for the scattering problem (see footnote 6). We believe that our present discussion for the bound-state problem is particularly streamlined. After the nonrecoil compensation, we encounter some terms from the pure Coulomb interaction which would be quite significant for the Lamb shift (of order  $\alpha^4 m_e^2/m_p$ ). Because of a special property of electrodynamics, a precisely compensating contribution occurs in the convection part of the one transverse photon exchange. This compensation was noted first in the work of Breit and Brown (1949). There it was observed in a rather offhand way as a property of certain integrals involving Dirac wave functions. The authors of the first papers on the order  $\alpha^5 m_e^2/m_p$  contributions to the Lamb shift do not mention this compensation at all. The reason is that they accepted the result of Breit and Brown for the lower-order term and simply calculated corrections to it. The compensation was discovered again by Grotch and Yennie (1967,1969) in a more transparent form.

In Sec. III.A we identify the kernels which must be evaluated to obtain all the contributions of the order of interest. We try to organize the perturbation kernels so that it is possible for the reader to see the origin of some of the older terms without becoming bogged down in the details of the higher-order ones. In Sec. III.B we describe a previously mentioned transformation to the covariant gauge kernels. Gauge corrections which are left over for the bound states either are too small to matter or they cancel awkward terms found in other contexts. In Sec. III.C, we explain the organization of the calculation so



that the disposition of the various contributions can be traced. In Sec. III.D we present the evaluation of the leading contribution (including reduced mass dependence), the Breit (1930) relativistic correction, and a small recoil term of the order of interest. Section III.E contains the calculation of the leading recoil correction, which involves one-loop kernels. Excluding radiative corrections, these are the only corrections to the Fermi splitting which were known before 1977. Rather than analyze them in their entirety there, we carry out the initial algebraic analysis of the graphs in Appendix B and study the resulting integrals in the main text. Parts which cannot be treated as a relativistic loop integral because they involve wave-function momenta are set aside to be treated in Sec. IV. They give contributions to the order of interest which can be evaluated rather straightforwardly.

In addition to the remainder of the one-loop kernels, we treat in Sec. IV other contributions arising from more complicated two-loop kernels. In this analysis it is essential that six related diagrams, corresponding to different ways of interconnecting the muon and electron lines with exchanged photons, be treated as a unit. This procedure is necessary in order to avoid spurious nonrecoil terms. In addition, in the intermediate momentum range ( $m_e < p < m_\mu$ ), it leads to a cancellation between these contributions (called the Caswell-Lepage cancellation) which prevents the occurrence of spurious terms of relative order  $\alpha^2(m_e/m_\mu)\ln(m_\mu/m_e)$ . In an earlier paper (Bodwin, Yennie, and Gregorio, 1978), this cancellation was discovered only at the end of a long calculation. The organization of that calculation obviously was not convenient for the avoidance of spurious terms and made the evaluation of the analytic terms considered here seem almost hopeless.

One of our objectives is to obtain the correct mass dependence of the coefficient of  $\ln\alpha$  so that the result is valid for positronium. This coefficient is of course already known from other recent work (Lepage, 1977; Bodwin and Yennie 1978). In obtaining it, we also calculate certain nonlogarithmic terms which may be applied to positronium. However, we have not been able to obtain all such terms analytically; at some point we are forced to use approximations based on the small mass ratio. To go further, a combination of analytic and numerical work is probably necessary. One calculation of this sort has recently been completed by Caswell and Lepage (1985) and another is in progress [Sapirstein (1984)].

In Sec. V, we work out the contribution of second order in the perturbation kernels. Due to the various refinements in our analysis, we need calculate only the term in which the hfs kernel acts twice. There are at least two Coulomb interactions between the kernels, the zero- and one-Coulomb interactions having been incorporated in individual kernels. Both  $S$  and  $D$  intermediate states must be summed over. Similar calculations have been done by Caswell and Lepage (1978a). There is not an exact correspondence between the contributions they calculated and those that appear in our formalism. However, we have calculated the additional contributions needed to

make a comparison, and have verified that our result agrees with theirs. Section VI gives a summary of the known results for the muonium hfs, together with a comparison with experiment. Positronium and hydrogen hfs are also briefly summarized.

This paper has several appendices. Appendix A contains a discussion of some general principles for estimating the orders of magnitude of various contributions. Appendix B, already mentioned, contains the algebraic analyses of the various sets of graphs for purposes of extracting the terms of interest and putting them into a convenient form for calculation. In Appendix C, we give a method for evaluating the necessary integrals analytically to the order of interest. Because this type of approach may have other applications, we describe it briefly here. Initially the integrals seem rather formidable, and straightforward procedures such as carrying out the energy integrations first lead rapidly to intractable expressions (possibly they could be worked out numerically). Some of the integrals that are basically nonrelativistic can be worked out by various tricks. The most difficult integrals are the seven-dimensional ones, with one energy variable and two spatial momenta. Here we use a rather indirect approach. The integral is first converted to a Feynman-parameter integral. Then simplifying approximations, valid to the order of interest, are made. At this point it is recognized that the result can be expressed as a combination of six-dimensional integrals (no energy variable) which reproduce the same Feynman-parameter integral. These integrals are easily evaluated in coordinate space. Since the same integrals occur in many contexts, summarizing tables are also given in Appendix C. The Grotch-Yennie treatment of the modified Dirac equation is outlined in Appendix D. In Appendix E, we construct the Bethe-Salpeter wave function from the results of Sec. II.A.

## II. FORMULATION OF AN EQUATION FOR BOUND-STATE QED CALCULATIONS

### A. General organization of bound-state perturbation theory

There exist many formulations of two-body bound-state theory in the literature, mostly based on the Bethe-Salpeter approach. They all give equivalent results if treated to the same level of accuracy, but they differ in considerable detail in overall organization and ease of calculation. The one to be described here seems especially adapted to the situation where there is a large mass ratio, but it can be used in the equal mass case to quite refined levels of contribution. Although much of the material to be presented below is "common knowledge" in the field, it seems important to include it in order to make precise the details of the calculation. Because of the application of current interest, we refer to the bound system as muonium; but many of our results are not limited to that system. For example, results which are not sensitive to the

nucleon structure are directly applicable to the hydrogen atom. These differences will be elaborated in the summary in Sec. VI. Throughout, we try to point out which results are also valid for positronium.

### 1. Zeroth-order treatment of bound states

We wish to choose an unperturbed problem that includes the basic nonrelativistic physics of the Schrödinger equation and as much of the relativistic physics as is feasible. There are many ways to accomplish this; all of them make use of the known solutions of the Schrödinger or Dirac equations with a given time-independent external potential. The method developed here is specialized to quantum electrodynamics, but some of the techniques should have a more general utility (for example, to quark-pair bound states). There are many ways to define the unperturbed problem; different choices simply produce different correction kernels. The trick is to make a choice that yields a fairly simple unperturbed problem *and* limits the number and complexity of the perturbation kernels. Furthermore, one wants the perturbations to yield truly small effects so that one can get reasonable results in finite order. For example, even though one particle mass may be much larger than the other one, it would be poor strategy to start with the infinite-mass limit. One should be able to get most of the reduced-mass effects at the unperturbed level. This turns out to be a somewhat subtle problem, and in fact there is no precise distinction between reduced mass and genuine dynamical recoil effects. Nevertheless, we will be able to obtain much of the mass dependence exactly, and most of our recoil corrections *look* dynamical.

Following the ideas of Salpeter and Bethe (1951), we arrive at the structure of our unperturbed problem by studying the two-particle four-point function. Since the Coulomb-interaction dominates the bound-state problem, we find it convenient to formulate the exchanged photon interaction in the Coulomb gauge. (Alternatively, one could formulate it in the Feynman gauge or some other convenient gauge, but still use the Coulomb potential as a starting point. The perturbation kernels would make up the differences in the end. Note that this would not preclude using a covariant gauge for radiative correction photons in the separate particle lines. Of course, a more careful discussion is necessary for positronium because of the annihilation diagrams.) The objective is to find the positions of the poles of the four-point function, which give us the energy (mass) eigenvalues of the two-particle system. Usually we are not interested in the wave function, except in some simplified approximation. Thus it is not useful to continue with the analysis of Salpeter and Bethe (1951), which leads to a four-dimensional integral equation for the wave function. We study instead the perturbation theory of the four-point function about some known reference. In fact, it will become clear from our work that the Bethe-Salpeter integral equation separates effects which should be treated together. For example, as

was already mentioned in the Introduction, it is necessary to treat together contributions arising from iterations of the kernels of the Bethe-Salpeter equation and those from higher-order kernels. If that is not done, spurious non-recoil effects occur, which cancel only when all contributions are added at the end. From either an analytic or a numerical point of view, it is undesirable to calculate spurious terms which are much larger than the ones of interest.

We first discuss the four-point function in the center-of-mass frame with pure Coulomb exchanges in the ladder approximation. (In other contexts one might use an alternative instantaneous potential, which is selected so as to incorporate as much of the basic physics as possible without sacrificing solubility.) Consider one iteration of the interaction. In momentum space each such iteration involves a four-dimensional loop integration. There are various ways to carry out the energy part of the loop integration, taking into account the fact that the Coulomb propagators are energy independent. The original approach of Salpeter (1952), which we do not reproduce here, was to carry out this integration explicitly. The result is quite complicated and not too useful for the refined calculations that are now being done. With further approximations, it can be reduced to a form that leads to the Schrödinger equation with reduced mass. One deficiency of the Salpeter equation is that it does not reduce to the Dirac equation as one mass goes to infinity. Rather, it contains a positive-energy (plane-wave) projection operator for the lighter particle. One can show that crossed Coulomb kernels restore the physics of the Dirac equation to given order in  $\alpha$ , but the procedure is quite cumbersome. There are other variants of this procedure in which a convenient propagator is written down in an *ad hoc* way. Examples are the wave functions of Caswell and Lepage (1978a) and Barbieri and Remiddi (1978).

Another recent approach, which is rather popular, is due to Gross (1969). In it, one of the particles (the heaviest) is put on mass shell. This approach does lead (after a few further minor approximations) to the Dirac equation for the lighter particle when the heavy mass becomes infinite. The nonrecoil relativistic corrections which remain are then easily seen to be cancelled by crossed graph contributions. A complication of this approach, which only becomes apparent at relatively refined stages of analysis, is that the exact unperturbed propagator depends on  $(\mathbf{p}^2 + m_\mu^2)^{1/2}$  (we call the heavy particle a muon). It is difficult to treat this dependence analytically, but it can be pushed into the perturbative kernels. In our experience, at some level the resulting perturbations lead to spurious divergences, which cancel only when several related kernels are added. Often perturbation kernels of quite different structure (some involving three-dimensional loops and others four-dimensional loops, for example) must be studied together to eliminate these spurious difficulties.

Our approach is quite close to the Gross equation treatment except that we first set the loop energy equal to a fixed value independent of the spatial momentum. At this point, the treatment is quite symmetric between the

two particles, so it would be equally applicable to positronium. The leading terms also reproduce the nonrelativistic physics with the correct reduced mass dependence. As is usual, our analysis is carried out in the center-of-mass frame ( $\mathbf{p}_e = -\mathbf{p}_\mu \equiv \mathbf{p}$ ). Before fixing the loop energy  $p_0$ , it is convenient to split the total energy  $E$  so that an amount  $E' + p_0$  is routed through the electron line and an amount  $E'' - p_0$  is routed through the muon line.<sup>7</sup> Here  $E = E' + E''$  and

$$E'^2 - m_e^2 = E''^2 - m_\mu^2 = -\gamma^2, \tag{2.1a}$$

which yields

$$E' = \frac{E^2 - m_\mu^2 + m_e^2}{2E}, \tag{2.1b}$$

$$E'' = \frac{E^2 - m_e^2 + m_\mu^2}{2E}.$$

For QED bound states, it turns out that

$$\gamma \approx \alpha m_r, \quad E' \approx m_e - \frac{\alpha^2 m_r^2}{2m_e}, \quad E'' \approx m_\mu - \frac{\alpha^2 m_r^2}{2m_\mu},$$

where  $m_r = m_e m_\mu / (m_e + m_\mu)$  is the reduced mass. Final results cannot depend on the momentum routing, of course, but the definition of the unperturbed propagator does. In our analysis,  $E'$  plays the role of the energy to be calculated. A small shift  $\Delta E'$  produces a shift in  $E$  given by

$$\Delta E = \Delta E' \frac{E}{E''}. \tag{2.1c}$$

With this choice, the product of electron and muon denominators takes on a particularly simple form

$$\frac{1}{D_e(p)D_\mu(-p)} = \frac{1}{2E} \frac{1}{p^2 - \gamma^2 + i\epsilon} \left[ \frac{2E''}{D_\mu(-p)} + \frac{2E'}{D_e(p)} \right], \tag{2.2a}$$

where

$$D_e(\pm p) = p^2 - \gamma^2 \pm 2E'p_0 + i\epsilon, \tag{2.2b}$$

$$D_\mu(\pm p) = p^2 - \gamma^2 \pm 2E''p_0 + i\epsilon.$$

In the very low momentum region  $|p^2 - \gamma^2| \ll |2m_e p_0|$ , the quantity in large parentheses in (2.2a) may be approximated by  $-2\pi i \delta(p_0)$ . Thus

$$(2.2a) \approx \frac{-2\pi i \delta(p_0)}{2E(-\mathbf{p}^2 - \gamma^2)}. \tag{2.2c}$$

Notice that this rearrangement produces a factor  $(2E)^{-1}$  rather than  $(2E'')^{-1}$ , which might have been guessed

<sup>7</sup>In effect, the choice of origin given here has been used previously by other authors (Todorov, 1971; and Austen and de Swart, 1983). For free particles with  $-\gamma^2 \rightarrow \mathbf{p}^2$ , it corresponds to having each particle on the mass shell.

from a study of the leading pole structure of the left side of (2.2a). It is the form (2.2c) that corresponds to the correct treatment of the reduced mass in the nonrelativistic region. Another way of writing (2.2a) which manifests the  $\delta$ -function term is

$$\frac{1}{D_e(p)D_\mu(-p)} = \frac{-2\pi i \delta(p_0)}{-2E(\mathbf{p}^2 + \gamma^2)} - \frac{1}{2E} \left[ \frac{1}{(p_0 + i\epsilon)D_e(p)} + \frac{1}{(-p_0 + i\epsilon)D_\mu(-p)} \right] \tag{2.2d}$$

[to show the equivalence, expand up  $p^2 - \gamma^2$  in the denominators inside the large parentheses of (2.2a), keeping the exact remainder].

Only the  $\delta(p_0)$  term is to be incorporated into our basic two particle propagator. Let us consider a number of examples for the particles (scalar or Dirac). The numerators are given (before fixing  $p_0$ ) in Table I. If we use the first term of (2.2d) and take the case of two scalars, we obtain the Schrödinger propagator for the two-particle system. Thus in scalar electrodynamics, we may combine the factor  $1/2E$  with the factors  $2E'2E''$  from the Coulomb interaction with the result  $2E'E''/E \approx 2m_r$ . The deviation from the reduced mass is small if  $\gamma \ll m_e, m_\mu$  in (2.1a). This is a good approximation for QED bound states, but note that the formalism does contain some relative-order  $\alpha^2$  corrections. In the Dirac-scalar or scalar-Dirac cases, the two-particle propagator becomes the Dirac propagator for one of the particles when  $p_0$  is fixed. In electrodynamics, the propagator is multiplied by  $E''/E$  or  $E'/E$ , respectively. The primary effect of this factor is to provide the correct reduced-mass effects; there are again corrections of relative order  $\alpha^2$  of course.

The Dirac-Dirac case, which is the one of greatest present interest, cannot be treated in the same manner. When  $p_0$  is fixed, the term  $-\alpha_e \cdot \mathbf{p} \alpha_\mu \cdot \mathbf{p}$  leads to divergent behavior at large momentum. However, it is interesting to note that the numerator is very close to that of the Breit two-particle propagator<sup>8</sup>

$$\frac{1}{E - H_e - H_\mu} = \frac{(E' + H_e)(E'' + H_\mu) - \mathbf{p}^2 - \gamma^2}{-2E(\mathbf{p}^2 + \gamma^2)},$$

where  $H_e = \alpha_e \cdot \mathbf{p} + \beta_e m_e$  and  $H_\mu = -\alpha_\mu \cdot \mathbf{p} + \beta_\mu m_\mu$ .

<sup>8</sup>The large-momentum difficulty with this propagator can be appreciated in the following way: Decompose it into various pieces using positive- and negative-energy projectors for the two particles. Terms with both positive- or both negative-energy projectors have an energy denominator which provides convergence at large momentum. This is the situation with Salpeter's (1952) original approach. However, the mixed terms have a denominator which tends to a constant at large momentum and does not produce convergence.

TABLE I. Various combinations of numerators for the two-particle propagator.

| $e \quad \mu$ | Numerator   |
|---------------|---|
| scalar-scalar | 1   |
| Dirac-scalar  | $(E' + \beta_e m_e + p_0 + \alpha_e \cdot \mathbf{p})$  |
| scalar-Dirac  | $(E'' + \beta_\mu m_\mu - p_0 - \alpha_\mu \cdot \mathbf{p})$   |
| Dirac-Dirac   | $(E' + \beta_e m_e + p_0 + \alpha_e \cdot \mathbf{p})(E'' + \beta_\mu m_\mu - p_0 - \alpha_\mu \cdot \mathbf{p})$ |

Perhaps there is some formulation which incorporates the relativistic and spin physics of this numerator for both particles, but we proceed to other simplifications which seem more practical. We can rewrite the two Dirac factors as

$$E'' + \beta_\mu m_\mu - p_0 - \alpha_\mu \cdot \mathbf{p} = \frac{1}{2}(E'' + m_\mu)(1 + \beta_\mu) + [\frac{1}{2}(E'' - m_\mu)(1 - \beta_\mu) - p_0 - \alpha_\mu \cdot \mathbf{p}] \quad (2.3a)$$

and

$$E' + \beta_e m_e + p_0 + \alpha_e \cdot \mathbf{p} = \frac{1}{2}(E' + m_e)(1 + \beta_e) + [\frac{1}{2}(E' - m_e)(1 - \beta_e) + p_0 + \alpha_e \cdot \mathbf{p}] \quad (2.3b)$$

The first terms on the right-hand side (rhs) of (2.3) dominate the nonrelativistic region, particularly for the heavier particle. We may choose to perturb about one or both of these terms. Let us describe these two possibilities. In the first, we take the first term of (2.3a) with the complete (2.3b), and fix  $p_0$  using the first term on the rhs of (2.2d); we then find

$$N_D \bar{S} = N_D \bar{s}(p)(-2\pi i)\delta(p_0), \quad (2.4a)$$

where

$$N_D = \frac{E'' + m_\mu}{2E}$$

and

$$\bar{s}(p) = \frac{\frac{1}{2}(1 + \beta_\mu)}{E' - \beta_e m_e - \alpha_e \cdot \mathbf{p}}$$

The normalizing factor  $N_D$ , which is approximately  $m_r/m_e$ , turns out to give the main reduced-mass effects. The two-body propagator  $\bar{s}$  is simply the large-component projector for the muon times the Dirac propagator for the electron. Some conventions for the propagators have been introduced here. They are used throughout the paper and are summarized in Table II.

There are two easily identifiable perturbations on (2.4a). One is the second term of (2.3a) with the original form of (2.2a) (left-hand side). The other is the first term of (2.3a) with the second term of (2.2d). The first of these perturbations is a recoil correction (vanishes as  $m_\mu \rightarrow \infty$ ); the second is not. However, as we show later, the nonrecoil perturbation is straightforwardly compensated and so need not be calculated.

In general, we represent diagrammatically the separation of the product of free propagators into a part containing  $\delta(p_0)$  (or some other prescription for fixing the loop energy) and perturbations as in Fig. 1(a). The heavy lines indicate the resulting three-dimensional propagator; and the  $R$  represents the remainder, which is to be treated as a perturbation. A perturbation scheme for dealing with this separation is presented in the next section.

The definition of the unperturbed problem in terms of (2.4a) is, unfortunately, no longer symmetric in the two particles. However, it is very well adapted to the situation where one mass ( $m_\mu$ ) is much greater than the other ( $m_e$ ). It is also useful for positronium through terms of order  $\alpha^2$  Ry and  $\alpha^3$  Ry. However, it may be preferable to have an explicitly symmetric form. Then we may choose the other possibility mentioned earlier in which we take the product of the first terms of (2.3) and fix  $p_0$  with the first term on the rhs of (2.2d)

$$N_S \bar{S}_S = N_S \bar{s}_S(p)(-2\pi i)\delta(p_0), \quad (2.4b)$$

where

$$N_S = \frac{(E'' + m_\mu)(E' + m_e)}{4Em_r}$$

TABLE II. Summary of notation used for Green's functions.

Barred lower-case letters are used to denote three-dimensional Green's functions; they have no  $p_0$  dependence.

Upper-case letters are used to denote four-dimensional Green's functions. An overbar is used to indicate a three-dimensional Green's function which has been promoted to four dimensions by appending a factor  $-2\pi i\delta(p_0)$ .

The letter  $s$  (either case) is used to denote a free propagator, while the letter  $g$  (either case) is used to denote a propagator with interactions.

The propagators used in this paper are

$\bar{s}, \bar{S}$ : Free three-dimensional two-particle propagator (2.4a).

$\bar{g}, \bar{G}$ : Three-dimensional propagator in an effective potential  $\mathcal{V}$  (2.5).

$S$ : Product of two free particle propagators  $[S_e S_\mu]$  (2.8).

$G$ : Complete four-point function with two-particle irreducible kernel  $K$  (2.8).

$\hat{G}$ : Four-point function based on  $\bar{G}$  perturbed by four-dimensional kernels  $N\hat{K}$  (2.11b).

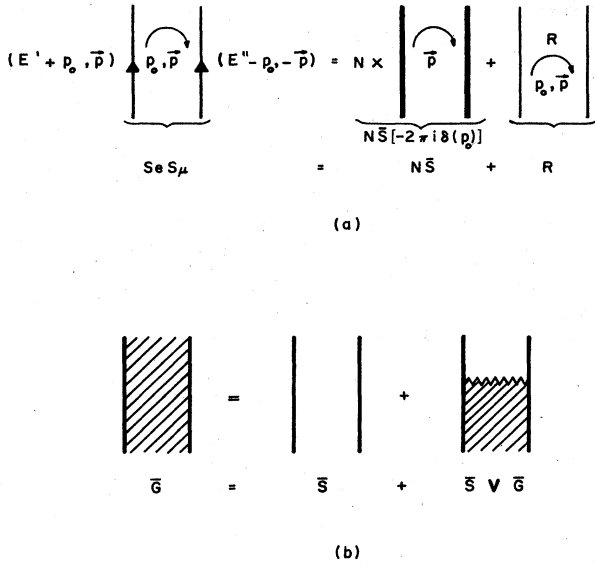


FIG. 1. (a). Graphical representation of the use of (2.2d). In this and in subsequent figures, the left fermion line represents the electron and the right one the muon. The lhs of the graphical equation represents the product of the free particle propagators with the specified energies and momenta. Some part of the numerator structure together with the first term of (2.2d) is represented by the first term on the rhs. Examples are (2.4a) and (2.4b) and the first term of (2.21b). The remainder is represented by the second term on the rhs. Our convention is to use heavy lines to indicate the fixing of  $p_0$  by the  $\delta$  function to give a simplified three-dimensional two-particle propagator. (b) Graphical representation of the integral equation for the complete three-dimensional propagator with an instantaneous potential. The complete propagator is represented by a shaded area between heavy lines and the potential by a saw-toothed line.

and

$$\bar{s}_S(p) = \frac{-2m_r}{p^2 + \gamma^2} \frac{1}{4} (1 + \beta_\mu)(1 + \beta_e).$$

The interpretation is obvious. This decomposition also takes the form represented by Fig. 1(a). Note that the factor  $N_S$  is very close to unity, except for very small binding corrections. As before, there are a number of perturbations, which we need not enumerate.

As a preliminary to the perturbation theory, we consider the three-dimensional Green's function  $\bar{g}$  defined by iterating either form of (2.4) with a potential  $V$ :

$$(N\bar{g}) = (N\bar{s}) + (N\bar{s})V(N\bar{g})$$

or

$$\bar{g} = \bar{s} + \bar{s}(NV)\bar{g}. \tag{2.5a}$$

For the choice (2.4a), this gives

$$(H_e + NV - E')\bar{g} = -\frac{1}{2}(1 + \beta_\mu)1. \tag{2.5b}$$

[In coordinate space  $1 \rightarrow \delta(x - x')$ .] As we show later, more physics can be incorporated into the basic wave equation if we use a different potential from the one ap-

pearing naturally. For the present, we do not detail these refinements, but simply replace  $NV$  by an effective potential  $\mathcal{V}$ . The Green's function  $\bar{g}$  produced by the interaction  $\mathcal{V}$  is represented diagrammatically as in Fig. 1(b).

Here it is important to note that  $\mathcal{V}$  depends on  $E'$  (rather weakly). For fixed  $E'$ , the eigenvalue equation (in the large component muon subspace) is

$$(H_e + \mathcal{V})|\bar{n}, E'\rangle = E'_n |\bar{n}, E'\rangle, \tag{2.6a}$$

and the Green's function can be written

$$\bar{g} = \frac{1}{2}(1 + \beta_\mu) \sum_n \frac{|\bar{n}, E'\rangle \langle \bar{n}, E'|}{E' - E'_n}, \tag{2.6b}$$

where the  $|\bar{n}, E'\rangle$  form a complete orthogonal set for each fixed value of  $E'$ . The bar notation for the states indicates that they are three dimensional. The same notation is used for functions which have been promoted to four-dimensional ones by appending a factor of  $\delta(p_0)$ . For later use, we note a subtlety here. The actual eigenvalues of the unperturbed problem are given by the zeros of the denominator of (2.6b), taking into account the dependence of  $E'_n$  on  $E'$ . Thus for the state  $n = 0$ , if the position of the pole is  $\tilde{E}'_0$ , we need to solve

$$\tilde{E}'_0 = E'_0(\tilde{E}'_0). \tag{2.7a}$$

In the vicinity  $E' \approx \tilde{E}'_0$ , we have

$$E' - E'_0(E') \approx (E' - \tilde{E}'_0) \left[ 1 - \frac{\partial E'_0}{\partial E'} \right]. \tag{2.7b}$$

The second factor on the rhs of this equation is sometimes absorbed into the normalization of  $|\bar{n}, \tilde{E}'_0\rangle$ :

$$|\bar{0}'\rangle = |\bar{0}\rangle \left[ 1 - \frac{\partial E'_0}{\partial E'} \right]^{-1/2}. \tag{2.7c}$$

It is easy to see that

$$\frac{\partial E'_0}{\partial E'} = \left\langle \bar{0} \left| \frac{\partial \mathcal{V}}{\partial E'} \right| \bar{0} \right\rangle. \tag{2.7d}$$

## 2. The perturbation expansion

In order to describe the calculation of the hyperfine structure precisely, we find it necessary to present the perturbation expansion in some detail. We make no claim that the following is original in principle, but probably the details have not been organized in quite the same way before.

The complete two-particle Green's function  $G$  satisfies

$$G = S + SKG, \tag{2.8a}$$

where  $S$  is the product of two free propagators and  $K$  is the complete two-particle irreducible kernel. We first split  $K$  into Coulomb interactions  $Q_c$  (instantaneous interaction  $V_c$  plus crossed Coulomb kernels) plus other kernels

$$K = Q_c + Q. \tag{2.8b}$$

Here  $Q$  contains all other interactions (transverse photon

exchanges, radiative corrections, etc.). It is assumed that the binding is produced by  $V_c$  and that the other terms, by themselves, do not lead to binding.

Our problem is to find a way to perturb about the three-dimensional solution described in the preceding section. First we must "promote" the equation for the Green's function to four-dimensional form in order to put it on the same footing as (2.8). To do this, we rewrite  $S$  as

$$S = N\bar{s}\delta + R = N\bar{S} + R. \quad (2.9a)$$

Here  $\bar{s}$  is a (free) three-dimensional Green's function and  $\delta [\equiv -2\pi i\delta(p_0)]$  represents the fixing of the loop energy according to the prescription discussed in the preceding section;  $R$  represents remainder terms which are to be treated as perturbations.  $\bar{S}$  is formally a four-dimensional Green's function, but one component is fixed by the  $\delta$ . In terms of  $\bar{S}$ , our "solvable three-dimensional problem" is

$$\begin{aligned} \bar{G} &= \bar{S} + \bar{S}\mathcal{V}\bar{G} \\ &= \bar{S} + \bar{G}\mathcal{V}\bar{S}. \end{aligned} \quad (2.9b)$$

$\mathcal{V}$  is the effective potential, mentioned in Sec. I, which is close to  $NV_c$  and which incorporates the dominant features of the bound-state problem. While (2.9b) is in the guise of a four-dimensional equation, its solution  $\bar{G}$  is of course known in terms of the related three-dimensional one.

Now we go through a series of steps to express the complete Green's function  $G$  in terms of the known function  $\bar{G}$ . This development is subject to considerable variation, depending on the ultimate objective. To obtain only the leading terms, one could pursue an apparently more straightforward procedure than the one to be presented here; but then the subsequent refinements would be somewhat more involved. Basically, the choice of procedure is a matter of taste. In the procedure to be presented here, the initial formal manipulation of the Green's functions may seem somewhat awkward, but it results in a more streamlined method for putting the kernels in the best form for actual computation.

In order to provide guidance to the reader, we first describe a perturbative analysis of  $G$ , ignoring the bound-state features of the problem, as well as the difference between  $\mathcal{V}$  and  $V_c$ . Suppose we iterate (2.8) to obtain  $G$  to all orders. Whenever an  $S$  occurs between two factors of  $Q_c$ , we use (2.9a). Contributions in which  $N\bar{S}$  appears between factors of  $V_c$  may be further rearranged using (2.9b) and summed up to produce the Green's function  $\bar{G}$ . Wherever an  $R$  appears between factors of  $Q_c$ , it produces a new type of kernel. Factors of  $S$  also occur between factors of  $Q_c$  and  $Q$  or between two factors of  $Q$ . This is where we have some freedom of choice. We could again apply (2.9a), obtaining one definition of the perturbation kernels; or we could keep  $S$  as it stands, obtaining a different definition. Experience has taught us that it is best to keep the complete  $S$  in these places. Ultimately, these differences have no consequences if we carry out our analysis carefully to a given order in  $\alpha$ . Terms that appear in lowest order in the perturbative kernels can be com-

bined with terms from second (or higher) order in an appropriate way so that one always obtains the same computational object in the end. The choice we make appears to lead most directly to kernels that are in a convenient form for calculation.

We now present the details of the perturbative analysis of  $G$ . Since the two inhomogeneous Green's-function equations (2.8a) and (2.9b) have different free parts, the procedure for relating them is somewhat subtle. The first step is to use (2.9a) in (2.8a). However, we do this only with the  $Q_c$  part of  $K$ ; the complete  $S$  is always used next to  $Q$ . Now we face the problem that we wish to expand about  $\bar{G}$ , not  $\bar{S}$ . To replace  $\bar{S}$  by  $\bar{G}$ , we act on our expression from the left with  $(1 + \bar{G}\mathcal{V})$  and use the second form of (2.9b). We then find

$$\begin{aligned} G &= N\bar{G} + R + RQ_cG + \bar{G}\mathcal{V}R + SQG \\ &\quad + \bar{G}N(\delta Q_c + Q_cRQ_c + Q_cSQ - \delta Q_cRQ_c - \delta Q_cSQ)G, \end{aligned} \quad (2.10a)$$

where we have introduced

$$\delta Q_c = Q_c - \mathcal{V}/N. \quad (2.10b)$$

We see that  $G$  is very close to  $N\bar{G}$ . The form (2.10a) is very convenient for iteration about that value. It is clear that that iteration produces a result of the form

$$G = \Lambda + (1 + \Gamma_l)N\hat{G}(1 + \Gamma_r), \quad (2.11a)$$

where  $\hat{G}$  has the form

$$\hat{G} = \bar{G} + \bar{G}\hat{K}\bar{G} + \bar{G}N\hat{K}\bar{G}N\hat{K}\bar{G} + \dots \quad (2.11b)$$

The form of  $\hat{K}$  depends on the details of the iteration procedure.

The procedure we use is the following. Where a factor  $QG$  occurs in (2.10a), first substitute for the  $G$  the form obtained by iterating (2.8a) with  $K$  given by (2.8b). Stop this iteration when a factor of  $Q_c$  is first encountered or when the order in  $Q$  becomes too high to be of interest. Now iterate (2.10) itself. One easily discovers that  $\hat{K}$  has the expansion

$$\begin{aligned} \hat{K} &= \delta Q_c + Q_cRQ_c + Q_cRQ_cRQ_c + Q_cSQSQ_c \\ &\quad + Q_cSQSQSQ_c + Q_cSQSQ_cRQ_c + \dots \end{aligned} \quad (2.11c)$$

The general structure is easy to describe. There is one two-particle irreducible term  $\delta Q_c$ . The two-particle reducible kernels must begin and end with  $Q_c$ , with any arrangement of  $Q$  and  $Q_c$  factors in between.  $Q$  is always separated from other factors by  $S$ , and any two adjacent factors of  $Q_c$  are separated by  $R$ . We could give expressions for  $\Lambda$  and the  $\Gamma$ 's here, but they are not necessary for the purpose of determining level shifts. The Bethe-Salpeter wave function can be constructed using the  $\Gamma$ 's; that is done in Appendix E.

The discussion of various kernels is given in subsequent sections. Here we describe how one finds a perturbation series for the energy levels. The energy levels are given by

the poles of  $G$ , or equivalently, those of  $\hat{G}$ . To find them, we consider the series (2.11b). We wish to use the eigenfunction expansion (2.6b) for a three-dimensional Green's function. This is done in an obvious way: the wave functions are "promoted" to four-dimensional ones which incorporate  $\delta$ . Then we take the expectation value of  $\hat{G}$  in the corresponding state to find

$$\begin{aligned} \langle \bar{0} | \hat{G} | \bar{0} \rangle &= \frac{1}{E' - E'_0} + \frac{\Sigma}{(E' - E'_0)^2} + \frac{\Sigma^2}{(E' - E'_0)^3} + \dots \\ &= \frac{1}{E' - E'_0 - \Sigma(E')}, \end{aligned} \quad (2.12a)$$

where

$$\begin{aligned} \Sigma(E') &= \langle \bar{0} | \hat{K} | \bar{0} \rangle N \\ &+ \sum_{n \neq 0} \frac{\langle \bar{0} | N \hat{K} | \bar{n} \rangle \langle \bar{n} | N \hat{K} | \bar{0} \rangle}{E' - E'_n} + \dots \end{aligned} \quad (2.12b)$$

The pole in  $E'$  is easily seen to be located at

$$\hat{E}'_0 \approx \tilde{E}'_0 + \Sigma(\tilde{E}'_0) \left[ 1 + \left\langle \bar{0} \left| \frac{\partial(\mathcal{V}' + N\hat{K})}{\partial E'} \right| \bar{0} \right\rangle_{E' = \tilde{E}'_0} \right], \quad (2.13a)$$

where  $\partial\mathcal{V}'/\partial E'$  enters through (2.7d). The energy shift is

$$\begin{aligned} \Delta E &\approx \langle \bar{0} | \hat{K} | \bar{0} \rangle \left[ 1 + \left\langle \bar{0} \left| \frac{\partial(\mathcal{V}' + N\hat{K})}{\partial E'} \right| \bar{0} \right\rangle_{E' = \tilde{E}'_0} \right] \\ &+ \sum_{n \neq 0} \frac{\langle \bar{0} | \hat{K} | \bar{n} \rangle \langle \bar{n} | \hat{K} | \bar{0} \rangle}{N^{-1}(E'_0 - E'_n)}, \end{aligned} \quad (2.13b)$$

where we have used (2.1c). Note that the factors of  $N$  have disappeared from most places; the denominator in the sum over states could be expressed as  $E_0 - E_n$ .

There is one final detail to be discussed. At the end of Sec. II.A.1, it was indicated that, in the three-dimensional problem, one can account for more of the physics by using a potential  $\mathcal{V}'$  that differs slightly from the Coulomb one. Thus we write

$$NV_c = \mathcal{V}' - NV'_c, \quad (2.14a)$$

so that

$$\delta Q_c = Q_c - V_c - V'_c. \quad (2.14b)$$

We choose  $\mathcal{V}'$  to be

$$\mathcal{V}' = V_c \left[ 1 - \frac{\beta_e m_e}{E} \right], \quad (2.15a)$$

so that

$$V'_c = V_c \frac{2(E' - \beta_e m_e)}{m_\mu + E''} - V_c \frac{\gamma^2}{(m_\mu + E'')^2}. \quad (2.15b)$$

The last term of (2.15b) is quite negligible for the hfs in muonium. As mentioned earlier, it is found that the main effects of the first term are cancelled by some residual perturbations from other kernels (see Sec. II.B). We also

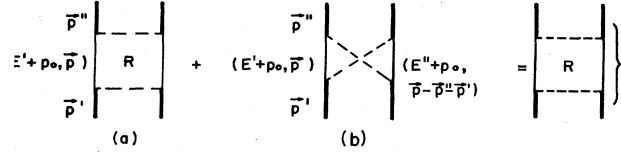


FIG. 2. (a) The perturbation kernel  $V_c R V_c$ , Coulomb exchanges being represented by dashed lines. (b) The simplest contribution to  $Q_c$  with two crossed Coulomb lines. In both graphs, the momenta in the electron lines have the same labeling. Thus the Coulomb photons have the same labeling, but the muon line four-momenta differ. This picture defines the meaning of the brace ({}): it represents the collection of graphs obtained by permuting the photon connections to the muon line in all possible ways. When an  $R$  occurs in such a diagram, it is to be used only in two-particle reducible structures.

note that replacing  $NV_c$  by  $\mathcal{V}'$  changes the order of magnitude of the factor  $\langle \bar{0} | \partial\mathcal{V}'/\partial E' | \bar{0} \rangle$  from  $\alpha^2 m_e/m_\mu$  to  $\alpha^2(m_e/m_\mu)^2$ , which makes it negligible in muonium for present purposes. With positronium, there seems to be no point in making such a change.

### B. Leading spin-independent kernels

We now study the simplest kernels  $\hat{K}$  which have a spin-independent piece. We start with the two-Coulomb kernels which are illustrated in Fig. 2.

First let us discuss the general features of the contribution  $V_c R V_c$ . For muonium,  $R$  is obtained by combining the Dirac-Dirac numerator of Table I with (2.2d) and dropping the product of the  $\delta$ -function term with the first term on the rhs of (2.3a). Recalling that  $\bar{G}$  contains the factor  $(1 + \beta_\mu)$ , we see that the  $-\alpha_\mu \cdot \mathbf{p}$  term in  $R$  does not contribute at all. It contributes when there are at least two  $R$  loops in succession, but then it yields contributions of relative order  $1/m_\mu^2$ . For the same reason, the term with a factor  $(1 - \beta_\mu)$  cannot contribute with a single  $R$  loop. Accordingly,  $R$  reduces to

$$\begin{aligned} &\frac{(E' + \beta_e m_e + p_0 + \alpha_e \cdot \mathbf{p})(m_\mu + E'' - p_0)}{2E} \\ &\times \left[ \frac{-1}{(-p_0 + i\epsilon)D_\mu(-p)} - \frac{1}{(p_0 + i\epsilon)D_e(p)} \right]. \end{aligned} \quad (2.16)$$

We note that this expression is symmetric in the two particles when it is taken between large components for the electron. (When the electron and muon are interchanged, the original expression may be restored by the variable change  $p_0 \rightarrow -p_0$ .) As mentioned earlier, the effects of this kernel do not vanish as  $m_\mu \rightarrow \infty$ , although it does contribute only to higher order in  $\alpha$ .<sup>9</sup>

Next we shall see how the crossed graph compensates the nonrecoil contribution from (2.16). Referring to Fig. 2(b), we see that the product of electron and muon factors for this kernel is

<sup>9</sup>We have not attempted to work it out. We expect it to be primarily of order  $\alpha^4$ , but with  $\ln\alpha$  dependence as well.



$$\frac{1}{E'+p_0-H_e(\mathbf{p})} \frac{1}{E''+p_0-H_\mu(\mathbf{p}-\mathbf{p}'-\mathbf{p}'')} \\ \doteq \frac{(E'+\beta_e m_e+p_0+\boldsymbol{\alpha}_e \cdot \mathbf{p})(E''+m_\mu+p_0)}{D_e(p)D_\mu(p-p'-p'')}, \quad (2.17a)$$

where we have taken into account the factors of  $(1+\beta_\mu)$  on either side of the expression and the fact that  $p'_0=p''_0=0$  in  $D_\mu$ . We want to rearrange (2.17a) so that it may be combined conveniently with (2.16). One way to do this is to rewrite the  $D_\mu$  factor

$$\frac{1}{D_\mu(p-p'-p'')} = \frac{1}{2E(p_0+i\epsilon)} \left[ 1 + \frac{D_e(p)}{D_\mu(p-p'-p'')} - \frac{(p-p'-p'')^2+p^2-2\gamma^2}{D_\mu(p-p'-p'')} \right], \quad (2.18)$$

so that (2.17a) becomes

$$\frac{(E'+\beta_e m_e+p_0+\boldsymbol{\alpha}_e \cdot \mathbf{p})(E''+m_\mu+p_0)}{2E} \left[ \frac{1}{(p_0+i\epsilon)D_e(p)} + \frac{1}{(p_0+i\epsilon)D_\mu(p-p'-p'')} \right. \\ \left. + \frac{-2(p-p'')(p-p')+(\mathbf{p}^2+\gamma^2)+(\mathbf{p}'^2+\gamma^2)}{(p_0+i\epsilon)D_\mu(p-p'-p'')D_e(p)} \right] \quad (2.17b)$$

We now observe that the nonrecoil pieces of (2.16) and (2.17b) cancel each other exactly. These are the terms with the  $D_e$  denominators and the factors of  $E''+m_\mu$  in the numerator. After this cancellation, we can set aside the  $\boldsymbol{\alpha}_e \cdot \mathbf{p}$  in the numerator and ignore the small components for most purposes. For the muonium hfs, corrections to these approximations cannot contribute to first order in (2.13b), while in second order they yield far too many powers of  $\alpha$  to be of interest at present. They do make a small contribution to the Lamb shift ( $\alpha^6 m_e^2/m_p$ ). At this point, we may make some transformations which manifest the symmetry under interchange of the two particles. In the second term in the large parentheses of (2.17b), we use the transformation  $\mathbf{p} \rightarrow \mathbf{p}'+\mathbf{p}''-\mathbf{p}$ . Because the potentials depend only on  $(\mathbf{p}'-\mathbf{p})^2$  and  $(\mathbf{p}-\mathbf{p}'')^2$ , this simply interchanges them, but it transforms  $D_\mu(p-p'-p'')$  to  $D_\mu(p)$ . Thus the sum of (2.16) and (2.17b) becomes

$$\frac{(E'+m_e+p_0)}{2E} \left[ \frac{2}{D_e(p)} - \frac{(E''+m_\mu-p_0)}{(-p_0+i\epsilon)D_\mu(-p)} + \frac{(E''+m_\mu+p_0)}{(p_0+i\epsilon)D_\mu(p)} \right. \\ \left. - \frac{(E''+m_\mu+p_0)[2p_0^2-2(\mathbf{p}-\mathbf{p}'') \cdot (\mathbf{p}-\mathbf{p}')-(\mathbf{p}'^2+\gamma^2)-(\mathbf{p}''^2+\gamma^2)]}{(p_0+i\epsilon)D_e(p)D_\mu(p-p'-p'')} \right]. \quad (2.19a)$$

This now vanishes for  $m_\mu \rightarrow \infty$ , so our objective has been accomplished.

By using symmetry and approximations, we can simplify (2.19a) further. Individual terms contain divergences in the  $p_0$  integration which cancel in the sum. In order to manipulate these terms separately, we must apply a regulator, which we choose to be even in  $p_0$ . Then, in the second term of the large parentheses, we make the variable change  $p_0 \rightarrow -p_0$ . In the last term, we neglect  $\mathbf{p}'$  and  $\mathbf{p}''$  in the denominator; the corrections would have an additional power of  $1/m_\mu$ . Then we find

$$\frac{E'+m_e+p_0}{ED_e(p)} + \frac{E''+m_\mu+p_0}{ED_\mu(p)} - \frac{(E'+m_e+p_0)(E''+m_\mu+p_0)p_0}{ED_e(p)D_\mu(p)} \\ + \frac{(E'+m_e+p_0)(E''+m_\mu+p_0)[2(\mathbf{p}-\mathbf{p}'') \cdot (\mathbf{p}-\mathbf{p}')+(\mathbf{p}^2+\gamma^2)+(\mathbf{p}'^2+\gamma^2)]}{2E(p_0+i\epsilon)D_e(p)D_\mu(p)}. \quad (2.19b)$$

The last term gives a significant contribution to the Lamb shift ( $\alpha^5 m_e^2/m_p$ ), but it is not important for the hfs. We do not study it further. The first three terms of (2.19b) give a more important contribution which must be treated properly for both the hfs and the Lamb shift. They may be rewritten

$$-\frac{p_0}{E} \left[ \frac{E''+m_\mu+p_0}{D_\mu(p)} - \frac{1}{p_0+i\epsilon} \right] \left[ \frac{E'+m_e+p_0}{D_e(p)} - \frac{1}{p_0+i\epsilon} \right] + \frac{1}{E(p_0+i\epsilon)} \approx -\frac{(\mathbf{p}^2+\gamma^2 p_0/2m_\mu)(\mathbf{p}^2+\gamma^2 p_0/2m_e)}{E(p_0+i\epsilon)D_\mu(p)D_e(p)} \\ + \frac{1}{E(p_0+i\epsilon)}. \quad (2.19c)$$

Now when the momentum is much smaller than the muon mass, the first term is of order  $1/m_\mu^2$ , so the second term dominates; and we can ignore the first term. Because of our choice of regulator, only terms symmetric in  $p_0$  survive. Thus, for contributions arising mainly from this region, we may approximate

$$(2.19c) \approx -\frac{2\pi i \delta(p_0)}{2E} \tag{2.19d}$$

When this piece of (2.19c) is combined with the Coulomb potentials, the result may be replaced by an effective interaction

$$V_{2c} = \frac{1}{2E} V_c^2 \tag{2.20}$$

This is to be understood in the following way: whenever the kernels pictured in Fig. 2 are taken between large electron components, their effects may be accounted for (in leading approximation) by taking  $V_{2c}$  as an effective term in  $\hat{K}$ . Now, the expectation value of (2.20) (between non-relativistic wave functions) yields a contribution of order  $\alpha^4 m_r^2/m_\mu$ . This would be a large contribution to the Lamb shift. In addition, it would contribute to the hfs to the present order of interest via terms which are second order in the kernels in (2.13b). Thus it is important to recognize that this contribution is, in fact, compensated. The compensating contributions are found in the simplest transverse photon kernel, which is illustrated in Fig. 3.

Figure 3 shows the decomposition of the one transverse photon kernel  $\hat{K}_T$  which results from (2.2d). Now we split up the unperturbed propagator  $S$  in a slightly different way than before, separating it into a part  $\bar{S}'$  in which we associate the complete muon numerator from Table I with the  $\delta(p_0)$  term and a new remainder  $R'$ . We could not do this in defining the unperturbed Green's function because it would have led to too singular an integral equation. Now, however, it is awkward to use  $\bar{S}$  in studying a specific kernel. Thus we have

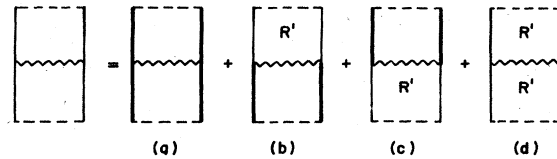


FIG. 3. Decomposition of the one transverse photon kernel  $\hat{K}_T = V_c S T S V_c$ . Here the one transverse photon interaction  $T$  is represented by a wavy line. The decomposition is based on applying (2.21a) to each loop.

$$S = N \bar{S}' + R' \tag{2.21a}$$

where

$$\bar{S}' = \frac{-2\pi i \delta(p_0)}{E' - \beta_e m_e - \alpha_e \cdot \mathbf{p}} \frac{E'' + \beta_\mu m_\mu - \alpha_\mu \cdot \mathbf{p}}{E'' + m_\mu} \tag{2.21b}$$

For the present, we consider only the contribution from the first term in (2.21a); the other terms yield higher-order contributions, which we will deal with later. The one transverse photon propagator, including lepton vertices, is given by

$$-4\pi\alpha \left[ \frac{\alpha_e \cdot \alpha_\mu}{q_0^2 - \mathbf{q}^2 + i\epsilon} - \frac{\alpha_e \cdot \mathbf{q} \alpha_\mu \cdot \mathbf{q}}{\mathbf{q}^2 (q_0^2 - \mathbf{q}^2 + i\epsilon)} \right] \tag{2.22}$$

where  $q_\lambda = p'_\lambda - p_\lambda$ . For the term being studied,  $q_0 = 0$ , of course.<sup>10</sup> Taking into account the factors  $(1 + \beta_\mu)$  contained in  $\bar{G}$ , we need keep only the terms even in  $\alpha_\mu$  in the spin reduction, i.e.,

$$(E'' + \beta_\mu m_\mu - \alpha_\mu \cdot \mathbf{p}') \alpha_\mu (E'' + \beta_\mu m_\mu - \alpha_\mu \cdot \mathbf{p}) \\ \doteq (E'' + m_\mu) [ -(\mathbf{p} + \mathbf{p}') - i\sigma_\mu \times (\mathbf{p}' - \mathbf{p}) ] \tag{2.23a}$$

Thus we need the matrix elements of the operator

$$\frac{4\pi\alpha}{E'' + m_\mu} N V_c \bar{S}'(\mathbf{p}') \left[ \frac{-\alpha_e \cdot (\mathbf{p}' + \mathbf{p})}{\mathbf{q}^2} + \frac{\alpha_e \cdot (\mathbf{p}' - \mathbf{p})(\mathbf{p}'^2 - \mathbf{p}^2)}{\mathbf{q}^4} + \frac{-i\alpha_e \cdot \sigma_\mu \times (\mathbf{p}' - \mathbf{p})}{\mathbf{q}^2} \right] \bar{S}(\mathbf{p}) N V_c \tag{2.23b}$$

The last term of (2.23b) (involving  $\sigma_\mu$ ) plays the leading role in the hfs; we treat it later. The piece of (2.23b) which is independent of the muon spin is known as the convection piece. Its contribution to  $\hat{K}$  will be denoted  $\hat{K}(\text{conv})$ . The inverse powers of  $\mathbf{q}^2$  occurring in (2.23) correspond to potentials in coordinate space in the following way:  $-4\pi\alpha/\mathbf{q}^2 = V_c(\mathbf{q})$ ,  $V_c(r) = -\alpha/r$ ; and  $-4\pi\alpha/\mathbf{q}^4 = -\frac{1}{2}W_c(\mathbf{q})$ ,  $W_c(r) = -\alpha r$ . (There is no problem in the Fourier transform of such a singular function, provided that one takes into account the factors of  $\mathbf{q}$  in the numerator.) Now we use  $\alpha_e \cdot \mathbf{p} = \bar{S}^{-1}(\mathbf{p}) + (E' - \beta_e m_e)$  to rearrange  $\hat{K}(\text{conv})$  to the following form (we approximate  $E'' \approx m_\mu$ ):

<sup>10</sup>Here we may point out a difference with other approaches. Had we followed the approach of Salpeter or Gross,  $q_0$  would have involved terms like  $m_\mu - (m_\mu^2 + \mathbf{p}^2)^{1/2}$  as well as contributions from the photon poles. These effects are small in the nonrelativistic region, but they lead to great complication in higher order. Separate terms are divergent, and the whole procedure is very awkward. In the present approach, by contrast, the corrections still contain four-dimensional integrals, but include no spurious divergences which must be compensated.

$$\begin{aligned} \hat{K}(\text{conv}) = & \frac{-4\pi\alpha}{2m_\mu} \left[ NV_c \bar{S}(\mathbf{p}') \left[ \frac{-1}{\mathbf{q}^2} - \frac{\mathbf{p}'^2 - \mathbf{p}^2}{\mathbf{q}^4} \right] NV_c + NV_c \left[ \frac{-1}{\mathbf{q}^2} + \frac{\mathbf{p}'^2 - \mathbf{p}^2}{\mathbf{q}^4} \right] \bar{S}(\mathbf{p}) NV_c \right] \\ & - \frac{4\pi\alpha}{2m_\mu} NV_c \bar{S}(\mathbf{p}') \frac{2(E' - \beta_e m_e)}{\mathbf{q}^2} \bar{S}(\mathbf{p}) NV_c . \end{aligned} \quad (2.23c)$$

Noting that this expression is ultimately to be sandwiched between propagators or wave functions, we find that it is convenient to rearrange certain factors in the following way:

$$\bar{S}(NV_c) = \bar{S} \mathcal{V}' - \bar{S}(NV'_c) = 1 - \bar{S} \bar{G}^{-1} - \bar{S}(NV'_c) , \quad (2.24)$$

where it is understood that  $\bar{G}^{-1}$  acts in the matrix space defined by the projector  $(1 + \beta_\mu)$ . To the orders of present interest, we can neglect the contributions arising from  $V'_c$  in (2.24). Then (2.23c) may be rearranged to the following form:

$$\begin{aligned} \hat{K}(\text{conv}) = & -\frac{2V_c^2}{2E} + V'_c - \frac{1}{4E} [V_c, [\mathbf{p}^2, W_c]] + \left[ \frac{V_c^2}{2E} - V'_c + \frac{1}{4E} V_c [\mathbf{p}^2, W_c] \right] \bar{S} \bar{G}^{-1} \\ & + \bar{G}^{-1} \bar{S} \left[ \frac{V_c^2}{2E} - V'_c + \frac{1}{2E} [W_c, \mathbf{p}^2] V_c \right] + \bar{G}^{-1} \bar{S} V'_c \bar{S} \bar{G}^{-1} . \end{aligned} \quad (2.23d)$$

Taking into account the identity

$$V_c^2 + \frac{1}{2} [V_c, [\mathbf{p}^2, W_c]] = 0 , \quad (2.25)$$

which is a special feature of the Coulomb interaction, we see an important cancellation between  $\hat{K}(\text{conv})$ ,  $-V'_c$  from (2.14b), and the effective interaction from the two-Coulomb contribution (2.20)

$$\left\langle \bar{0} \left| \hat{K}(\text{conv}) - V'_c + \frac{V_c^2}{2E} \right| \bar{0} \right\rangle = 0 . \quad (2.26a)$$

In the case of matrix elements between the ground state and excited states the cancellation is incomplete [because of the  $\bar{G}^{-1}$  terms in (2.23e)] and we are left with

$$\left\langle \bar{0} \left| \hat{K}(\text{conv}) - V'_c + \frac{V_c^2}{2E} \right| \bar{n} \right\rangle = \left\langle \bar{0} \left| \left[ \frac{V_c^2}{2E} - V'_c + \frac{V_c}{4E} [\mathbf{p}^2, W_c] \right] \bar{S} \right| \bar{n} \right\rangle (\tilde{E}'_0 - \tilde{E}'_n) . \quad (2.26b)$$

To see the effect of this term, consider the sum over states in (2.13b). The factor  $(\tilde{E}'_0 - \tilde{E}'_n)$  cancels the energy denominator. Then we can use closure to carry out the sum, taking care to subtract the term where  $n=0$ . The sum over all  $n$  yields an effective contribution to  $\hat{K}$

$$\left\langle \bar{0} \left| \left[ \frac{V_c^2}{2E} - V'_c + \frac{V_c}{4E} [\mathbf{p}^2, W_c] \right] N \bar{S} \hat{K} \right| \bar{0} \right\rangle . \quad (2.27)$$

To obtain a contribution to the hfs, we can use the one-transverse photon piece of  $\hat{K}$ . While (2.27) contains terms of the order of interest, none of them needs to be calculated. As noted in Sec. III.A.2, a contribution cancelling the  $-V'_c$  term arises from the reorganization of the kernels. The term involving  $W_c$  is cancelled by a gauge correction term in Sec. III.B. Finally, the  $V_c^2/2E$  term is cancelled by a term from VOV, as discussed in Sec. IV.B.3.

The  $n=0$  term subtraction is just cancelled by the  $\partial \hat{K} / \partial E'$  term from (2.13b). When we differentiate (2.23e) with respect to  $E'$  and take the ground-state expectation value, the derivative must act on  $\bar{G}^{-1}$  to give a significant contribution; but then it produces a result which precisely cancels the  $n=0$  subtraction term. This type of cancellation is undoubtedly familiar to the experienced reader.

### III. ORGANIZATION OF THE CALCULATION AND EVALUATION OF THE LEADING-ORDER AND ONE-LOOP CONTRIBUTIONS TO HFS

This is a transitional section from the general formalism developed in Sec. II to the more detailed calculations of the hyperfine splitting which will be discussed in subsequent sections. The first objective is to transform the perturbation scheme developed in Sec. II.A into a practical one for actual calculations. The first step in this direction is to group together graphs which have a related photonic structure. The groupings consist of graphs which have the same photon connections on the electron line and all permutations of connections on the muon line. The different groups are labeled by the sequence of connections on the electron line. To the present order of interest, it turns out that we need graphs with up to two four-dimensional loops. We may use the  $N\bar{S}/R$  separation to rearrange the original Feynman integrals, as illustrated in Fig. 3. However, in practice it is awkward to implement this separation by a revised set of Feynman rules, so we use it only to simplify graphs with more than two four-dimensional loops. Thus, in the final calculation, we retain the left-hand side (lhs) of Fig. 3. However, the rearrangement is

instructive, because it shows that this complete kernel contains three types of terms, characterized by different numbers of intrinsic  $p_0$  integrations. For instance, the first one [Fig. 3(a)], with no intrinsic  $p_0$  integration, contains the leading contribution, complete with the correct reduced-mass dependence and Breit (1930) relativistic correction. It is worked out as a separate calculation in Sec. III.D; we refer to it as the  $V$  term. In a similar way, we want ultimately to isolate terms which are associated primarily with one intrinsic  $p_0$  integration such as the second and third terms of Fig. 3, and those with two intrinsic  $p_0$  integrations such as the fourth term of Fig. 3. The ones in Fig. 3 are by themselves not convenient, because they contain spurious nonrecoil contributions and other difficulties. Before isolating terms with different numbers of loops, we reorganize the kernels into convenient sets which are conveniently treated together.

The reorganization of the kernels is carried out in Sec. III.A. This aspect of the analysis is not specific to QED bound states, but the next step is. In Sec. III.B, in order to circumvent the complications of noncovariant denominators and the transversality condition, we rewrite the kernels in terms of covariant gauge photons. This is not a gauge transformation, because the external lines are not on mass shell. Nevertheless, the differences between the kernels in the two gauges turns out to be small, and where they cannot be neglected they nicely compensate terms which arise elsewhere in the analysis. Having arranged the kernels into convenient sets, we proceed to the isolation of contributions which correspond to differing numbers of  $p_0$  integrations in Sec. III.C.

Our next objective in this section is to rederive the historic results in this field, namely, the leading-order result [basically the Fermi (1930) splitting as improved by the Breit (1930) relativistic correction] and the leading recoil correction (Arnowitt, 1953; and Newcomb and Salpeter, 1955). This work is done in Secs. III.D and III.E. To our knowledge, this paper is the first one which incorporates these results together with the higher-order terms in one formalism. In previous treatments the problem has been that approximations that worked well for certain contributions, say, the recoil correction, were extremely awkward for others, such as the Breit correction. Since we wish to make these results accessible to a casual reader, we do not deal with all the complications from the start. On the other hand, the expressions for the leading terms generally contain many higher-order contributions as well. We do not wish to calculate these leading terms so crudely that we must deal with extra complications in order to recover higher-order terms later on. The organization of the calculation developed in Sec. III.C seems to be well adapted to these goals.

### A. Reorganization of the kernels

By our seemingly awkward treatment of the perturbation expansion, we have actually simplified the next step of the analysis, which is to rearrange and group the ker-

nels so as to streamline the actual calculation. Had we followed a different procedure, we could have arrived at this point by bringing together various contributions which contain the same type of interactions, but have their origins in different orders of perturbation theory. It is here that the awkwardness would enter had we followed a simpler procedure earlier.

#### 1. Pure Coulomb kernels

As has already been shown, certain combinations of contributions manifest cancellations which make their sum of higher order in  $m_e/m_\mu$  than the individual terms. A simple example is provided by the nonrecoil contributions of Fig. 2, whose cancellation is shown in (2.19). The noncancelling terms cannot contribute to the hfs in first-order perturbation theory, and their contribution in second order was shown in Sec. II.B to be canceled by a piece of the convection part of Fig. 3.

All the perturbation kernels involving three Coulomb interactions are shown in Fig. 4. For the complete collection there is again a cancellation of nonrecoil pieces. In fact, the first three terms and the last three terms separately exhibit this cancellation. The actual orders of magnitude of the energy shifts arising from the three Coulomb interaction graphs are  $\alpha^6 m_e^2/m_p$  for the Lamb shift and  $\alpha^6 m_e^3/m_\mu^2$  for the hfs. Since these are of sufficiently high order for the present level of interest, we do not continue the discussion to higher numbers of loops, which would lead to more powers of  $\alpha$ . Actually, we do not calculate these terms as they stand. It proves much more convenient to transform our kernels to a covariant gauge before doing any calculations.

Having identified the perturbative contributions to the hfs, we now wish to reexpress the perturbation kernels in terms of ordinary Feynman integrals by using (2.9a) in reverse. [This is *not* a step backward in the analysis, since it was necessary to use the decomposition (2.9a) in the four-point function in order to obtain a sensible perturbation expansion in the first place.] The result is illustrated in Fig. 5. The first term on the rhs of this graphical equation is denoted CCC. The combination of terms on the rhs is a genuine four-dimensional two-loop integral; but individual terms contain lower-order contributions.

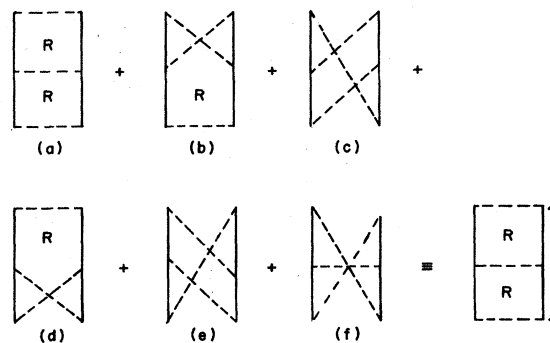


FIG. 4. The set of three-Coulomb kernels, with its shorthand notation.

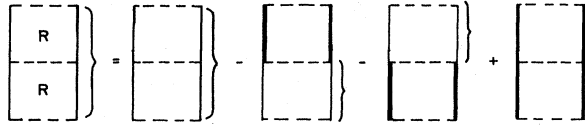


FIG. 5. Rearrangement of the three-Coulomb kernels using (2.2d).

2. Transverse photon kernels

We have already discussed the features of the one transverse photon kernel shown in Fig. 3. As we explained, this kernel is to be kept intact for the calculation of the hfs to first order in the kernels. For the contribution which is second order in the kernels, only the first term is important for the present order of interest. The role of the spin-independent part is described in Sec. II.B. The second-order contribution of the spin-dependent piece is evaluated in Sec. V. Because of our particular definition of the unperturbed wave function and the way we arrange the perturbation expansion, this is the only kernel which must be treated in second-order perturbation theory. Of course, if one calculates to higher order in  $m_e/m_\mu$  or  $\alpha$ , a huge number of additional contributions appear.

In Fig. 6 are shown several kernels involving one trans-

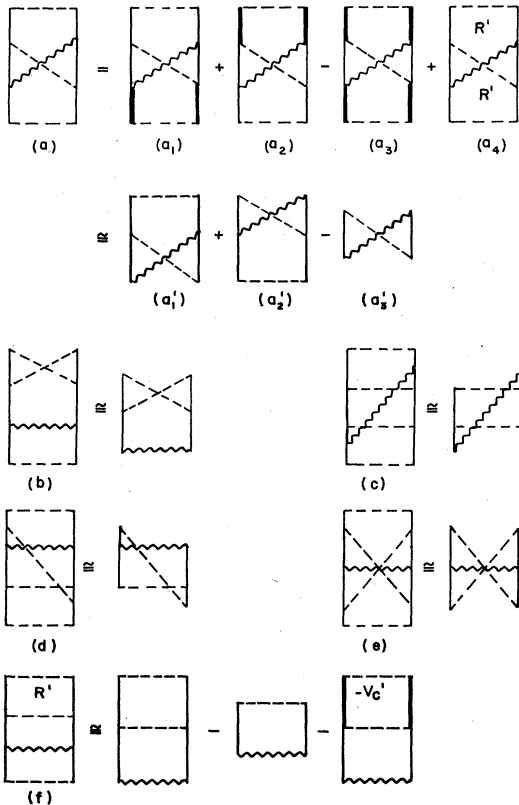


FIG. 6. Some graphs with one transverse photon, broken down into contributions with various numbers of intrinsic four-dimensional loops. Graphs with more than two intrinsic four-dimensional loops such as (a<sub>4</sub>), and others not shown, are ignored in the present work. The approximation sign represents the dropping of terms beyond the order of interest, as described in the text.

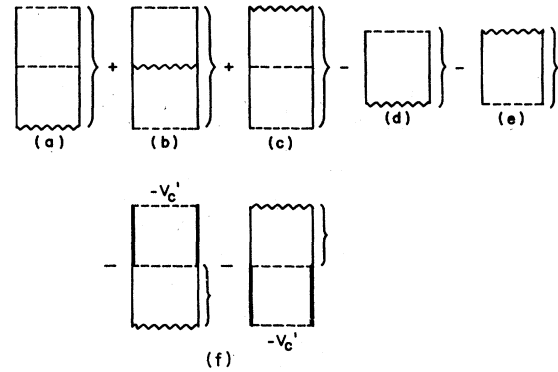


FIG. 7. The result of the rearrangement of the contributions with one T exchange. The principal contributions [(a)–(e)] are labeled TCC, CTC, CCT, –TC, and –CT, respectively. The final two are small contributions, which are compensated by terms having a different origin, as explained in the text.

verse photon, along with rearrangements that make use of the  $N\bar{S}'/R'$  separation to isolate the pieces with more than two intrinsic  $p_0$  integrations. The latter are to be discarded at the present level of accuracy. Figure 6(a) shows the decomposition of a kernel with crossed Coulomb and transverse photon lines. Figure 6(a<sub>4</sub>) is the piece to be discarded. Further simplification is possible. If we apply (2.24) to the heavy-line subgraphs in the first three terms, we find that the  $V'_c$  terms cancel to the order of interest, so that only the 1 terms remain. Thus, to the order of interest, we may erase the heavy-line subgraphs. Such approximations are denoted with an approximation sign in our graphical equations. Thus all the remaining contributions illustrated in Fig. 6 have a leading part which contains two four-dimensional integrations. Note that in the approximate form of Fig. 6(f), a term involving  $-V'_c$  is left over after we use (2.24). Although it is not compensated by contributions from other single transverse photon kernels, it is canceled by the  $-V'_c$  term in (2.27) to the order of interest. Thus it need not be evaluated.

Next we group together all contributions having the same order of attachment of the photon lines to the electron line—including all orderings of the photons on the muon line. The result is illustrated in Fig. 7. The terms in this expression are labeled TCC, CTC, CCT, –TC, and –CT, respectively. It is instructive to verify, by using the  $N\bar{S}'/R'$  separation, that the leading term and one intrinsic  $p_0$  loop contributions are contained the correct number of times in this combination. Note that had we been calculating only through the one loop level we would

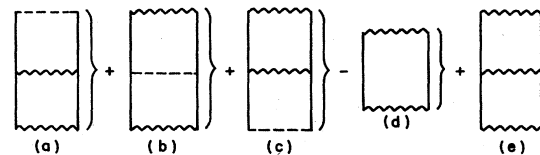


FIG. 8. Contributions with two or more transverse photons. They are labeled as follows. (a) TTC; (b) TCT; (c) CTT; (d) –TT; and (e) TTT.

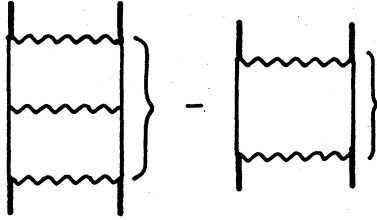


FIG. 9. The complete set of diagrams which is to be calculated. Here, the wavy lines represent  $T + C$  originally, but after the discussion of Sec. III.B, they become  $V + O$ . All contributions, including leading order, one loop, and two loops are included with exactly the right weight. The subtraction removes any overcounting of contributions in the first term.

have obtained simply the combination  $TC + CT - T$ .

Following a similar procedure, one can easily discover the set of diagrams involving two or three transverse photons. They are shown in Fig. 8. It is important to note that  $V'_c$  terms have again canceled to the order of interest. By combining Figs. 5, 7, and 8, one can rewrite the entire set of kernels which must be calculated in lowest-order perturbation theory as shown in Fig. 9. Here it is understood that each photon line stands for the sum of Coulomb and transverse photon interactions. (Note that although the pure Coulomb terms written here are different from the original expressions, they give the same hfs contributions.)

### 3. A further useful redefinition

Let us review briefly the meaning of Fig. 9. The kernels shown represent "raw" Feynman integrals with external momenta supplied by the wave functions. The heavy lines represent wave functions which include the full Dirac structure of the electron and a context-dependent spin structure for the muon. If the external muon line is next to an original  $Q_c$  kernel, our decomposition of  $S$  would have been into  $N\bar{S} + R$ ; and only large muon components would be present in the wave function. On the other hand, if the external muon line is next to an original  $Q$  kernel, the decomposition  $S = N\bar{S}' + R'$  would provide small muon components. It is awkward to keep track of this distinction.

To avoid the problem of treating the muon spin structure differently for different graphs, we simply insert the muon small components in all the wave functions and consider any corrections separately. It turns out that all effects due to these corrections cancel to the order of interest. This is due primarily to the subtraction structure of Fig. 9. Let us look at some examples. Consider the effect of putting the muon small components in after the final  $C$  in both  $CTC$  and  $-TC$ . The subtraction amounts to having an  $R'$  in the  $CT$  loop of  $CTC$  in combination with small muon components in the final wave function; the result is of too high an order of  $\alpha$  to be of interest at present. Muon small components after the final  $C$  in  $TCC$  or  $TTC$  or in both wave functions of  $CTC$  directly

yield too high an order. In pure Coulomb terms,  $CCC$  contributes to the hfs, but  $-CC$  does not. When the muon small components are introduced in the wave function, new hfs contributions are introduced as well, but they cancel between  $CCC$  and  $-CC$  to the order of interest. We have achieved the objective of a uniform treatment of the muon spin structure for all the graphs. However, if one were to pursue terms beyond the present order of interest, it would be necessary to reexamine this discussion.

### B. The transformation of the kernels to a covariant gauge

We note that if the external lines of Fig. 9 were on mass shell we would have a gauge-invariant set of contributions. For the nonrelativistic region of the wave functions, the external legs are nearly on mass shell. Thus we may transform to a gauge covariant kernel, producing only a small correction. This correction is actually canceled by a term having a different origin, and hence needs never to be calculated.

Kernels constructed from  $T$  and  $C$  are awkward because they contain both noncovariant and covariant denominators and have a complicated numerator structure due to the transversality of  $T$ . These photon factors, including the lepton-photon vertices, are given by

$$C = \frac{4\pi\alpha}{-q^2} = \frac{4\pi\alpha}{q^2} - \frac{4\pi\alpha q_0^2}{q^2 q^2} = O - \delta O, \tag{3.1a}$$

$$T = 4\pi\alpha \left[ -\frac{\alpha_e \cdot \alpha_\mu}{q^2} + \frac{\mathbf{q} \cdot \alpha_e \mathbf{q} \cdot \alpha_\mu}{q^2 q^2} \right] = 4\pi\alpha \left[ -\frac{\alpha_e \cdot \alpha_\mu}{q^2} + \frac{q_0^2}{q^2 q^2} + \frac{(\alpha_e \cdot \mathbf{q} - q_0)\alpha_\mu \cdot \mathbf{q}}{q^2 q^2} + \frac{q_0(\alpha_\mu \cdot \mathbf{q} - q_0)}{q^2 q^2} \right] = V + \delta O + \xi_e + \xi_\mu. \tag{3.1b}$$

Now the combination in Fig. 9 is really  $(T + C, T + C, T + C) - (T + C, T + C)$ . In this combination

$$T + C = V + O + \xi_e + \xi_\mu, \tag{3.1c}$$

where  $\xi_e$  and  $\xi_\mu$  have the structure of gauge terms in one leg or the other. If these were scattering diagrams with the external legs of the kernel on mass shell, these terms would yield zero.

As an example of the treatment of gauge terms, consider the case in which one of them occurs next to the final wave function on the muon leg. This leads to a structure

$$-Q_0\psi^\dagger(\mathbf{p}') \left[ 1 - \frac{\boldsymbol{\alpha}_\mu \cdot \mathbf{p}'}{E'' + m_\mu} \right] [\boldsymbol{\alpha}_\mu \cdot (\mathbf{p}' - \mathbf{Q}) + Q_0] \\ \times \frac{1}{E'' - Q_0 - \beta_\mu m_\mu + \boldsymbol{\alpha}_\mu \cdot \mathbf{Q}} \dots,$$

which may be rearranged to give an "end term"

$$+ Q_0\psi^\dagger(\mathbf{p}') \frac{\gamma^2 + \mathbf{p}'^2}{E'' + m_\mu} \frac{1}{E'' - Q_0 - \beta_\mu m_\mu + \boldsymbol{\alpha}_\mu \cdot \mathbf{Q}} \dots \quad (3.2)$$

plus a term which participates in a pairwise cancellation in the usual way and needs not be shown explicitly. The four vector  $Q_\lambda$  is "generic"; it depends on the other photon insertions occurring in the muon line. A similar end term (but with opposite overall sign) results for the case in which the gauge term occurs next to the initial wave function. These end terms would be zero if the muon were on mass shell.

Now we discuss various situations in which these end terms on the muon leg can occur, taking into account the subtraction of the one-loop from the two-loop graphs. Suppose we have an end term next to the final wave function that comes from the combination  $OX\xi_\mu - X\xi_\mu$ , where  $X$  is any of the photon types in (3.1c). We claim that the result is of too high an order in  $\alpha$  for present consideration. The reason is that there are necessarily three loops of relativistic electron momenta because of the subtraction and the factor of  $Q_0$  which prevents the occurrence of a factor  $\delta(Q_0)$ . In case the end term is next to the initial wave function, a similar argument holds for  $X\xi_\mu O - X\xi_\mu$ . This takes care of all the cases in which the subtraction terms can participate. The case of an initial-state end term coming from  $OX\xi_\mu$  also involves three relativistic electron loops, as do any other terms involving  $\xi_\mu$  which have not just been discussed.

The gauge term for the electron must be examined with a bit more care, since it does not have a factor of  $q_0$  to kill terms proportional to  $\delta(q_0)$ . It can give a contribution to the order of interest only in conjunction with the  $\delta(p_0)$  pieces of the muon propagators (2.2c). Thus it cannot contribute for any graphs where there is a  $p_0$  in the numerator. As in the previous case, terms of the order of interest cancel because of the subtraction of the one-loop from the two-loop contributions. The only remaining possibility is a ladder structure with  $V$  followed by  $O$  followed by an end term on the electron side. If we are to have two factors of  $\delta(p_0)$ , the photons must not be crossed. Taking into account the spin structure of the wave function (momentum  $\mathbf{p}''$ ) and the adjacent muon propagator (momentum  $\mathbf{p}'$ ), we find for the muon factor the structure

$$\left[ \frac{1 + \beta_\mu}{2} - \frac{\boldsymbol{\alpha}_\mu \cdot \mathbf{p}''}{E'' + m_\mu} \right] \boldsymbol{\alpha}_\mu \cdot (\mathbf{p}'' - \mathbf{p}') \frac{E'' + \beta_\mu m_\mu - \boldsymbol{\alpha}_\mu \cdot \mathbf{p}'}{2E} \\ \doteq - \frac{\mathbf{p}''^2 - \mathbf{p}'^2}{2E}.$$

The notation ( $\doteq$ ) introduced here means that the two ex-

pressions lead to the same hfs content to the order of interest. The end term on the electron side yields

$$\psi^\dagger(\mathbf{p}'')(\boldsymbol{\alpha}_e \cdot \mathbf{p}'' + \beta_e m_e - E') = \psi^\dagger(\mathbf{p}'') \mathcal{V} \\ \doteq -\psi^\dagger(\mathbf{p}'') NV_c,$$

and we find an effective contribution to  $\hat{K}$

$$\frac{-1}{4E} \langle 0 | NV_c[\mathbf{p}^2, W_c] N \bar{S} \hat{K}_{\text{spin}} | 0 \rangle, \quad (3.3)$$

where  $\hat{K}_{\text{spin}}$  is the leading order piece of  $\hat{K}$  which contributes to the hfs. This contribution just cancels the last term in (2.27), as mentioned there.

The contributions involving more than one  $\xi_e$  photon are too small to enter at the present order of interest. With two  $\xi_e$  photons and a  $V$  photon, or three  $\xi_e$  photons, this is straightforward to check. With two  $\xi_e$  photons and an  $O$  photon, one must first make use of the pairwise cancellation between the three photon graphs. Then there remain contributions in which one end term is associated with each wave function. These contributions are easily seen to be too small.

The previous graphs should now be reinterpreted with  $T \rightarrow V$  and  $C \rightarrow O$ . From now on, we label a given set of graphs according to the order of insertion of the photons on the electron line, starting with  $\psi$  and ending with  $\psi^\dagger$ .

### C. Overview of the organization of the calculation

As indicated previously, our next goal is to arrange the calculation so that contributions which are predominantly identified with different numbers of  $p_0$  integrations are isolated. The leading contribution  $V$  has already been mentioned. Next we want to define the "additional" contributions from one  $p_0$ -loop graphs which will be called [VO], [OV], and [VV]. Finally, the "additional" contributions from two  $p_0$ -loop graphs will be called [VOO], [OVO], [OOV], [VVO], [VOV], [OVV], [OOO], and [VVV]. The purpose of this section is to give an overview of this procedure, which is basically an analysis of the algebraic structure of the integrands of the different sets of graphs, with details provided in Appendix B. There is a certain amount of arbitrariness about the definitions of these different expressions; it is necessary only to make certain that all the relevant contributions from Fig. 9 are retained. At a minimum, for example, [VO] should incorporate *all* one  $p_0$ -loop effects, but there is no need to exclude effects of higher order. Our definition does include such effects, which arise naturally from that particular set of graphs. In practice the lower-order expressions are quite simple and it is easy to retain such higher-order terms (this is not true in certain other formalisms which we explored). As we proceed to higher orders the expressions of course become more complicated, but it is possible to make many approximations in which contributions beyond the current order of interest (of order 0.1 ppm)



can be dropped. While ideally we would keep all terms which contribute in positronium, that would be much more difficult than the work presented here (and probably would require some numerical analysis). Instead, we retain all terms which yield  $\alpha^2 \ln \alpha E_F$  correctly for positronium, but drop nonlogarithmic contributions in that order.

To isolate the reader from some of the distracting details, we confine the analysis of the integrands of the various kernels to Appendix B, and display only the resulting integrals in the main text. Most details of the evaluation of the integrals are also confined to an appendix, but the strategy is explained in the main text. We hope that this format will be helpful to readers who may wish to pursue the subject at different levels.

We recognize that each graphical contribution may be decomposed into pieces in various ways. Certain parts of each graphical contribution may not be straightforwardly treated at the same level at which the main terms are considered. For example, they may be of higher order than the one of current interest; then they can be discarded. More difficult are terms which lead to a spurious (too low) order if treated by themselves; they are properly treated only when combined with terms which arise from apparently more complicated graphs. For the most part, we avoid discussing these complications in the main text, but deal with them adequately in Appendix B. As we proceed from simpler to more complicated graphical sets, we notice that the more complicated ones include contributions already treated at a previous level. In fact, as described below, the subtraction indicated in Fig. 9 assures that each individual contribution is correctly counted. We identify these and deal only with the truly new effects. To indicate this, we use the following notation: A square bracket ([ ]) around the symbol for a set of graphs represents a "new" contribution associated with that set. Thus a set of graphs is generally decomposed into a number of terms: ones found previously in simpler graphs plus the new ones which arise. In addition, there are "other terms" which cannot be properly treated within the set of graphs. Here we note these terms (with  $\dots$ ), but do not describe them in detail or how they ultimately cancel.

The dominant term arises from Fig. 3(a). Schematically, we write

$$\text{Fig. 3(a)} \rightarrow V + \dots \quad (3.4)$$

The precise definition of  $V$  and its calculation are given in Sec. III.D.

If we were proceeding only to the one-loop level, we would have to work out the combination  $VO + OV + VV - V$ , in place of Fig. 9. The  $VO$  term is identified with Fig. 7(d) (with  $+$  sign). Its decomposition is given in Appendix B Sec. 1.a, where it is shown that

$$VO \approx V + [VO] + \dots, \quad (3.5a)$$

where  $[VO]$  is the new term to be calculated. The "other terms" noted here are not negligible, but they participate in various cancellations as explained in the appendix. We

could further separate  $[VO]$  into one- and two-loop contributions:

$$[VO] = [VO]_1 + [VO]_2. \quad (3.5b)$$

The one-loop part is studied in Sec. III.E and the two-loop part in Sec. IV.A.1. Of course, if we are interested only in terms of relative accuracy  $\alpha m_e/m_\mu$ ,  $[VO]_2$  can be ignored.

The structure of  $VOO$  is analyzed in Appendix B Sec. 1.b. It is found to have the form

$$VOO \approx V + [VO] + [VOO] + \dots \quad (3.6)$$

The  $[VOO]$  calculation is described in Sec. IV.A.2.  $OOV$  has a similar form.

The structure of  $OVO$  is analyzed in Appendix B Sec. 1.c. The result can be expressed as

$$OVO \approx V + [VO] + [OV] + [OVO] + \dots \quad (3.7)$$

The  $[OVO]$  calculation is described in Sec. IV.A.3.

The collection of terms involving one  $V$  exchange is now seen to be

$$\begin{aligned} VOO + OVO + OOV - VO - OV \\ \approx V + [VO] + [OV] + [VOO] + [OVO] + [OOV]. \end{aligned} \quad (3.8)$$

Most of the "other terms" largely cancel among themselves; some are canceled by terms having their origin in two  $V$  exchange contributions.

The algebraic rearrangement of  $VV$  is given in Appendix B Sec. 2.a with the result

$$VV = [VV] + \dots \quad (3.9a)$$

It is convenient to split this into one- and two-loop pieces:

$$[VV] = [VV]_1 + [VV]_2. \quad (3.9b)$$

The one-loop piece is treated in Sec. III.E, and the two-loop calculation is explained in Sec. IV.B.1.

$VVO$  is analyzed in Appendix B Sec. 2.b, and it decomposes as follows:

$$VVO = [VV] + [VVO] + \dots, \quad (3.10)$$

with a similar breakup for  $OVV$ . The calculation of  $[VVO]$  is described in Sec. IV.B.2.

As outlined in Appendix B Sec. 2.c,  $VOV$  has the decomposition

$$VOV = [VOV] + \dots \quad (3.11)$$

The calculation of  $[VOV]$  is described in Sec. IV.B.3. The sum of two  $V$  terms is

$$\begin{aligned} VVO + VOV + OOV - VV \approx [VV] + [VVO] \\ + [VOV] + [OVV], \end{aligned} \quad (3.12)$$

where we have omitted "other terms," which cancel against ones from the one- $V$  graphs.

The  $OOO$  and  $VVV$  contributions are relatively straightforward and self-contained. The algebraic analy-

ses are in Appendix B Secs. 3 and 4, and the calculations are described in Secs. IV.C and IV.D.

#### D. Leading order contribution to hfs

The largest contribution to the hyperfine splitting is provided by the kernel illustrated in Fig. 3(a). Its muon factor is given by the last term of (2.23b). To define the standard one-V contribution, we use (2.24) and absorb the  $\bar{S}\mathcal{V}$  factors into the wave function, dropping the  $V'_c$  terms. At this point we find

$$\hat{K}_T \doteq \frac{4\pi\alpha}{E'' + m_\mu} \frac{-i\sigma_\mu \times \mathbf{q} \cdot \boldsymbol{\alpha}_e}{q^2}, \quad (3.13)$$

where  $\mathbf{q} = \mathbf{p}' - \mathbf{p}$ . The expectation value of this kernel is to be evaluated using the Grotch-Yennie equation wave functions derived in Appendix D. The latter may be expressed in terms of the usual Dirac bound-state wave functions  $\chi_n$  for the Coulomb potential. They are (for the ground state)

$$\psi_0 = \left[ \frac{1 + \beta_e m_e/E}{1 + f_0(\bar{\alpha}) m_e/E} \right]^{1/2} \chi_0(\bar{m}_e \bar{\alpha} r, \bar{\alpha}), \quad (3.14)$$

where

$$\bar{\alpha} = (1 - m_e^2/E^2)^{1/2},$$

$$\bar{m}_e = m_e(1 - E_0'/E)/(1 - m_e^2/E^2)^{1/2},$$

and

$$f_0(\bar{\alpha}) = (1 - \bar{\alpha}^2)^{1/2}.$$

Other details are in Appendix D. Note that  $\bar{\alpha}\bar{m}_e \approx m_r$ , where  $m_r = m_e m_\mu / (m_e + m_\mu)$ . The error made in the approximation is of relative order  $\alpha^2 m_e / m_\mu$  and is important only as a correction to the leading term. It need not be considered with terms which are intrinsically smaller.

We find that the first-order contribution of (3.13) to the hfs is given by

$$\Delta E(T) = \frac{4\pi\alpha}{m_\mu} \frac{(1 - m_e^2/E^2)^{1/2}}{1 + f_0(\bar{\alpha}) m_e/E} \left\langle \frac{-i\sigma_\mu \times \mathbf{q} \cdot \boldsymbol{\alpha}_e}{q^2} \right\rangle, \quad (3.15a)$$

where we use  $E'' + m_\mu \approx 2m_\mu$ , with an error of relative order  $\gamma^2/m_\mu^2$ , which is not presently of interest for muonium, but would be for positronium. Here the expectation value is to be taken with the  $\chi_0$  factor of (3.14). Except for the modified parameters, this is precisely the calculation done by Breit (1930); it gives the result for the hfs

$$\begin{aligned} \Delta E(T) &= \frac{8}{3} \frac{\alpha \bar{\alpha}^3 \bar{m}_e^2 (1 - m_e^2/E^2)^{1/2}}{m_\mu (1 + f_0(\bar{\alpha}) m_e/E)} \left[ 1 + \frac{3}{2} \bar{\alpha}^2 + O(\bar{\alpha}^4) \right] \\ &\doteq E_F \left[ \frac{m_e + m_\mu}{E} \right]^3 \left( 1 + \frac{3}{2} \bar{\alpha}^2 \right) \\ &\doteq E_F \left[ 1 + \frac{3}{2} \alpha^2 + \frac{3\gamma^2}{2m_e m_\mu} \right], \end{aligned} \quad (3.15b)$$

where  $E_F$  is given by (1.1), and terms of relative order  $\alpha^2(m_e/m_\mu)^2$  have been dropped.

Incidentally, most earlier treatments of the relativistic two-body problem do not connect with the Dirac equation in a simple way. This means that the  $\frac{3}{2}\alpha^2$  term in (3.15b), which arises from the structure of the Dirac wave function (noninteger radial dependence), is difficult to obtain. In fact, it appears as a second-order (in  $\hat{K}$ ) contribution in the other treatments. To our knowledge, the present treatment is the only unified discussion of  $O(\alpha^2)$  recoil and nonrecoil contributions.

We can indicate here how the radiative corrections can be incorporated into this result. The electron's anomalous moment interaction has a different structure from (3.13), but its leading contribution can be determined by taking the nonrelativistic approximation for the large components of the wave function. This effect can be incorporated by adding the electron anomaly  $a_e$  to the parentheses of (3.15b). Beyond that, the dynamical structure of the magnetic moment operator and other radiative corrections to the electron and photon lines explore the relativistic momentum range for the electron. These add terms of order  $\alpha^2$  to the parentheses. Finally, since the muon's anomalous moment represents a modification of the static magnetic field at this level, its effect can be incorporated by multiplying the new parentheses—except for the  $\gamma^2/m_e m_\mu$  term—by the factor  $1 + a_\mu$ . We do not include the recoil term because it is probably inconsistent to do so; in any case, the result would be too small to matter at the present time.

#### E. The one-loop contribution to the hfs

In this section we initiate the evaluation of the contributions [VO], [OV], and [VV]. The dominant terms, which are wave-function insensitive, are studied in this section. The remaining terms have operators containing powers of wave-function momenta. They are discussed in the next section. To follow the calculation in complete detail, the reader should first refer to Appendix B Secs. 1.a and 2.a. The purpose of the appendix is to take the raw Feynman expressions for the integrands of the kernels and rearrange them into a convenient form for the actual calculations, dropping terms which are too small to be of interest at the present time. We believe it should be possible to get an overview of the method without studying the appendix in detail; and here we simply outline the approach. As has been emphasized repeatedly, separate graphs yield various spurious terms which compensate when they are added. It is important to make these compensations manifest in the integrands before the calculation is carried through. Without studying the appendix in complete detail, one can easily see how the nonrecoil cancellations occur in [VO] in the steps leading to Eqs. (B5). It would be very easy to start from (B5) and confirm the calculation to the level of accuracy of this section; that could be done with rather crude approximations. Howev-

er, to proceed to the next order in  $\alpha$ , it is necessary to develop some relatively refined rearrangements. The ones presented in the appendix were arrived at after much trial and error. In the initial stages of our work, we made a rather brute-force expansion in inverse powers of  $m_\mu$ . However, this has the disadvantage that the results are automatically invalid for positronium. Subsequently it was found that some (but not all) terms could be treated analytically in a mass-symmetric way. Clearly, it is desirable to preserve the mass symmetry as long as possible, provided that doing so does not increase the computational labor unduly. We make these remarks since the

motivation of the steps used in the appendix may not always be completely obvious.

As just mentioned, we try to keep the symmetry between electron and muon so that the results can be applied to positronium. However, it sometimes becomes necessary, for ease of calculation, to expand in the small mass ratio  $m_e/m_\mu$ . We try to point this out in the appendix, and in the main text, whenever it is done. Except for relative-order  $\alpha^2$  nonlogarithmic terms, our final results are valid for positronium.

We find after removing the V contribution from VO that the energy shift associated with [VO] is

$$\Delta E([\text{VO}]) = -(4\pi\alpha)^2 \frac{\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle}{m_\mu^2 - m_e^2} \int \frac{d^3p' d^4p d^3r}{-(2\pi)^{10}i} \frac{\phi_{\text{nr}}^\dagger(\mathbf{p}') \phi_{\text{nr}}(\mathbf{r})}{[(p' - p)^2 + i\epsilon][(p - r)^2 + i\epsilon]} \{I_e([\text{VO}]) - I_\mu([\text{VO}])\}, \quad (3.16)$$

where the function  $I_\beta([\text{VO}])$  is derived in Appendix B Sec. 1.a.  $\phi_{\text{nr}}$  is the nonrelativistic ground-state wave function which is an adequate approximation for our present purposes. Some important properties of  $\phi_{\text{nr}}$  are given in (3.17) below. The form of (3.16) is significant; the specific electron and muon dependences are separated from each other. Ultimately, this makes it possible to carry out these integrals analytically to the order of interest so that the result may be applied to positronium.  $I_\beta([\text{VO}])$  consists of several terms, most of which depend on wave-function momenta explicitly. Only one of these giving the leading contribution is presented in this section. It is the one which is least sensitive to the wave-function dependence and we refer to it as the "one-loop" term. It is given by

$$I_\beta([\text{VO}]_1) = \frac{-(p' - p)^2 (p - r)^2}{2(p_0 + i\epsilon)^2 D_\beta(p)},$$

where  $D_\beta(p)$  is defined in (2.2b). The other parts of  $I_\beta([\text{VO}])$  are given in Sec. IV.A.1. Note that  $p'_0 = r_0 = 0$ .

Although  $I_\beta([\text{VO}]_1)$  still has some wave-function dependence, it is a particularly useful form, because the factor  $(p - p')^2$  cancels a denominator from a photon propagator. In the other terms of  $I_\beta([\text{VO}])$ , the wave-function dependence occurs in a more intrinsic way. After using  $(p - p')^2$  to cancel the photon propagator, we carry out the  $p'$  integration, using the first of

$$\int \phi_{\text{nr}}(\mathbf{p}') \frac{d^3p'}{(2\pi)^3} = \tilde{\phi}_{\text{nr}}(0) \quad (3.17a)$$

and

$$\int \frac{\phi_{\text{nr}}(\mathbf{p}')}{(p' - p)^2} \frac{d^3p'}{(2\pi)^3} = \frac{\tilde{\phi}_{\text{nr}}(0)}{p^2 + \gamma^2}. \quad (3.17b)$$

(The second of these depends on the specific form of the ground-state wave function.)  $\tilde{\phi}_{\text{nr}}(0)$  is the spatial wave function at the origin, which for the ground state has the value  $(\gamma^3/\pi)^{1/2}$ . Next we use

$$\frac{(p - r)^2}{p_0^2 - (p - r)^2 + i\epsilon} = -1 + \frac{p_0^2}{p_0^2 - (p - r)^2 + i\epsilon}. \quad (3.18a)$$

With the  $-1$ , the  $\mathbf{r}$  integration can be carried out using (3.17a). The remaining  $\mathbf{p}$  integration is easily performed and we find for the integral in (3.16)

$$-1 : \frac{\gamma^3}{8\pi^3} \ln \frac{m_\mu}{m_e}.$$

Terms which are of higher order in  $\alpha$  than those of interest have been dropped.

With the second term of (3.18a), we "decouple" the  $\mathbf{r}$  integration using the convenient rearrangement

$$\frac{1}{p_0^2 - (p - r)^2 + i\epsilon} = \frac{1}{p^2 - \gamma^2 + i\epsilon} + \left[ \frac{1}{p_0^2 - (p - r)^2 + i\epsilon} - \frac{1}{p^2 - \gamma^2 + i\epsilon} \right]. \quad (3.18b)$$

This rearrangement is used frequently in subsequent work. The particular separation made has the important property that the second term frequently cancels because of (3.17). The first term of (3.18b) is easily worked out to the order of interest and gives the result for the integral

$$\text{decoupled piece of (3.18b): } \frac{\gamma^3}{16\pi^3} \ln \frac{m_\mu}{m_e} - \frac{(m_\mu - m_e)\gamma^4}{32m_e m_\mu \pi^2}.$$

The second term of (3.18b) is called a "decoupling correction." To evaluate it, we first put the two pieces over a common denominator, producing a numerator  $r^2 - 2\mathbf{p} \cdot \mathbf{r} - \gamma^2$ . Special integral tables are given in Appendix C to handle contributions like this. The  $r^2 - 2\mathbf{p} \cdot \mathbf{r}$  term may be expressed in terms of  $K_{13}$  after a relabeling

of variables. The  $-\gamma^2$  term emphasizes very low momenta, so we may neglect  $p^2 - \gamma^2$  in  $D_\beta$ . Then, using symmetry, we find

$$\frac{1}{p^2 - \gamma^2 + 2E_\beta p_0 + i\epsilon} \approx \frac{1}{2E_\beta(p_0 + i\epsilon)} \doteq -\frac{\pi i \delta(p_0)}{2E_\beta}. \quad (3.19)$$

[The approximation (3.19) is used frequently in other parts of the calculation.] The remaining work is now quite trivial and we obtain for the integral

$$\text{decoupling correction} : -\frac{(m_\mu - m_e)\gamma^4}{32m_e m_\mu \pi^2}.$$

$$\Delta E([VV]_1) = 3(4\pi\alpha)^2 \frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle \int \frac{d^3 p' d^4 p d^3 r}{-(2\pi)^{10} i} \frac{\phi_{nr}^\dagger(p') \phi_{nr}(r) (p^2 - \gamma^2)^2}{[(p' - p)^2 + i\epsilon] D_e(p) [(p - r)^2 + i\epsilon]} \left[ \frac{1}{D_\mu(p)} - \frac{1}{D_\mu(-p)} \right]. \quad (3.21)$$

The first step in the evaluation is to use (3.18b) to separate each photon propagator into a part in which the wave function decouples and a decoupling correction. The piece of (3.21) in which both wave functions decouple is easily evaluated by first doing the  $p_0$  integration. The only subtlety is that the  $\gamma^2$  dependence in the denominators yields a small contribution which could easily be overlooked. The result for the decoupled part is

$$\Delta E([VV]_1; \text{dec}) = E_F \left[ \frac{3\alpha}{\pi} \frac{m_e m_\mu}{m_\mu^2 - m_e^2} \ln \frac{m_\mu}{m_e} - \frac{3}{2} \frac{\gamma^2}{m_e m_\mu} \right]. \quad (3.22a)$$

Examination shows that to the order of interest, we need keep only the combinations of a decoupled term for one photon and a correction for the other. Two decoupling corrections together yield too high an order. After using Eq. (B22) to rearrange the expression, we find that the necessary integrals are given by  $-K_1[(p'^2 - 2\mathbf{p} \cdot \mathbf{p}' - \gamma^2)(p^2 + \gamma^2)]$  and  $-2K_7(p'^2 - 2\mathbf{p} \cdot \mathbf{p}' - \gamma^2)$ . This adds  $-3$  to the coefficient of the last term of (3.22), yielding the complete result to the order of interest.

$$\Delta E([VV]_1) = E_F \left[ \frac{3\alpha}{\pi} \frac{m_e m_\mu}{m_\mu^2 - m_e^2} \ln \frac{m_\mu}{m_e} - \frac{9}{2} \frac{\gamma^2}{m_e m_\mu} \right]. \quad (3.22b)$$

This completes the calculation of the one-loop terms.

#### IV. EVALUATION OF THE TWO-LOOP CONTRIBUTIONS

In Sec. III.E we discussed the one-loop contributions associated with [VO], [OV], and [VV]. These had a piece for which the wave functions could be (nearly) decoupled and integrated separately using (3.17a). At that time, oth-

Combining the results of all the integrations and doubling to take into account OV, we find

$$\Delta E([VO]_1 + [OV]_1) = E_F \left[ -\frac{6\alpha}{\pi} \frac{m_e m_\mu}{m_\mu^2 - m_e^2} \ln \frac{m_\mu}{m_e} + \frac{2\gamma^2}{m_\mu m_e} \right]. \quad (3.20)$$

Note that the factor involving the muon's anomalous moment is divided out of the Fermi splitting; it would be incorrect to incorporate it.

The energy shift associated with the one-loop part of [VV], as derived in Appendix B Sec. 2.a, is given by

er contributions were set aside to be treated as two-loop effects, because they depended in a more intrinsic way on the wave-function momentum. The various contributions involving two intrinsic four-dimensional loops are denoted according to the arrangement of V- and O-type photons coupled to the electron line: [OOO], [VOO], [OVO], [OOV], [VVO], [VOV], [OVV], and [VVV]. To find these contributions, we follow the procedure described in Sec. III.C. This work, which is essential and somewhat laborious, is relegated to Appendix B; but we make some general remarks about it here.

An important feature of the two-loop contributions is a cancellation in the intermediate momentum range ( $m_e \leq p \leq m_\mu$ ) which improves the convergence by one degree. We refer to this important feature of the permuted graphs as the Caswell-Lepage cancellation (Caswell and Lepage, 1978b). As explained by them, the cancellation arises in the hfs (not the Lamb shift) when the three-photon connections to the electron line are reversed. The reason is that if the electron mass is neglected in this region, the spin structures in the two related diagrams cancel. This implies that the first noncancelling contribution has an additional factor of  $m_e$  in the numerator. The implications of this are (a) any contribution whose integrand is  $O(1/m_\mu^2)$  in this region converges and does not produce a factor of  $\ln(m_\mu/m_e)$ , as it would for separate graphs; and (b) any contribution with more inverse powers of  $m_\mu$  can diverge in this region, but it cuts off for momenta greater than  $m_\mu$  (provided all contributions are treated together) and produces a result of order  $1/m_\mu^3$  (possibly with logarithms). The consequence of this is that when we wish to expand in inverse powers of  $m_\mu$  and retain terms through  $1/m_\mu^2$ , we may simply expand up the two-loop integrands. We have been able to treat terms yielding  $\ln\alpha$  in a mass-symmetric way so that we can verify the known contribution for positronium; however, we have not found a way to obtain a complete analytic result for positronium to the order of interest. We should em-

phasize that the Caswell-Lepage cancellation does not apply to one-loop contributions where, as we have seen,  $\ln(m_\mu/m_e)$  factors do occur. In that case the two related graphs add rather than cancel.

In our approach, we permute the photon connections in the muon legs in all ways. This clearly produces the same effect as permuting in the electron leg, and the Caswell-Lepage cancellation is valid, although the form is slightly different: if the electron mass is neglected in the intermediate momentum region, the complete integrand is an odd function under simultaneous inversion of both loop momenta. Again, this means that the actual integral must contain a factor of the electron mass and the convergence is improved by one power. Although the cancellation is manifest, it is occasionally convenient to analyze individual terms for which it is not. That may be done by using some consistent regularization, e.g., dimensional, which may be applied to the separate terms. It turns out that by means of some computational tricks, the necessary integrals can be worked out analytically. These techniques are described in Appendix C; and a set of useful integrals, to which we refer frequently, is also given there.

Our analysis is presented at several levels. In the main text, the basic organization of the calculation is presented in enough detail that its general nature can be perceived and the "bookkeeping" aspects followed. As much as possible, actual details are confined to the appendices. The first step there is to study the muon factor for each permuted set and remove the terms which have already been calculated in the leading or one-loop terms. The remaining contributions are examined to find any which may contribute  $\ln\alpha$  to the order of interest; these are to be treated in such a way that the correct mass-symmetric coefficient is obtained. All other terms are expanded to order  $1/m_\mu^2$ . The resulting muon factors are presented in the main text and the complete integrands are broken

down into various types of terms. The details of the method of integration are presented in Appendix C.

### A. Contributions involving one V

We give here a brief description of some features of the analysis of the muon factors given in Appendix B. In the VO contribution, a piece associated with the leading-order V is easily identified in the Feynman integrand and removed, as is a  $V_c$  term from (2.24) which is set aside and ultimately compensated for by a piece of VV. Most of the remainder is denoted as [VO] and is incorporated in (3.16) and (4.1). However, there are two additional terms which are recognized to be "spurious" and are set aside. As explained in Sec. III.D, VOO, OVO, and OOV are analyzed to identify their V, [VO], and [OV] parts plus the new contributions [VOO], [OVO], and [OOV] plus some additional spurious terms which are set aside. While this may seem to be an awkward procedure, it is actually quite convenient. One analyzes the "raw" Feynman integrands for the two-loop kernels and easily identifies the previously calculated one-loop terms to be subtracted. In addition, some terms of higher order than those of present interest are identified and discarded. Only the terms which need to be evaluated at the present order of interest are displayed in the main text.

#### 1. Remainder from [VO]

In Sec. III.E we worked out the leading one-loop contribution which arises from [VO]. Our immediate goal here is to work out the other terms which were not considered previously. For convenience, we reproduce the expression for the [VO] contribution here:

$$\Delta E([VO]) = - (4\pi\alpha)^2 \frac{\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle}{m_\mu^2 - m_e^2} \int \frac{d^3p' d^4p d^3r}{-(2\pi)^{10} i} \frac{\phi_{nr}^\dagger(\mathbf{p}') \phi_{nr}(\mathbf{r})}{[(p' - p)^2 + i\epsilon][(p - r)^2 + i\epsilon]} \{I_e([VO]) - I_\mu([VO])\}. \quad (4.1)$$

The part of  $I_\beta([VO])$  not previously considered is

$$I_\beta([VO]_2) = \left[ \frac{-[\mathbf{p}' \cdot (\mathbf{p}' - \mathbf{p}) - \mathbf{r} \cdot \mathbf{p}' + \mathbf{p} \cdot \mathbf{r}](\mathbf{p} - \mathbf{r})^2}{2(p_0 + i\epsilon)^2} + (\mathbf{p}' - \mathbf{r}) \cdot (\mathbf{p} - \mathbf{r}) + \frac{(\mathbf{p}' - \mathbf{r})^2 p_0}{4E_\beta} \right] \frac{1}{D_\beta(p)}.$$

We consider in succession all the terms from  $I_\beta([VO]_2)$ , providing them with a convenient identifying label.

(i)  $-(\mathbf{p} - \mathbf{r})^2 (\mathbf{p}'^2 - \mathbf{p} \cdot \mathbf{p}')$ . We again use (3.18) to reorganize the expression. We first argue briefly that the last term of (3.18b) does not contribute to the order of interest. For it we may neglect  $p^2 - \gamma^2$  in  $D_\beta$ ; corrections to this are of higher order than is of present interest. Then using (3.19) and (3.17), we find that the two pieces of the last term of (3.18b) cancel. This illustrates the advantage of this particular method of decoupling, which we use often. Now we proceed to the important terms. We recombine the remaining two pieces of (3.18) and use (3.17a) to eliminate the  $\mathbf{r}$  integration. The result of these

approximations is to replace  $(\mathbf{p} - \mathbf{r})^2$  in the original integrand by  $p^2 + \gamma^2$  (in two places). The  $p^2$  in the numerator is given by the integral table ( $K_{15}[p^2(\mathbf{p}^2 - \mathbf{p} \cdot \mathbf{p}')$ , with interchange of arguments). The  $\gamma^2$  term is worked out as follows. We note that the integral must produce inverse powers of  $\gamma$  in order to arrive at a contribution of the desired order. This means that very small momentum must be emphasized and hence we may neglect the  $p^2 - \gamma^2$  terms in the denominators of (4.1). Having done that, we note that because of the symmetry of the integral, the factor  $1/(p_0 + i\epsilon)^3$  may be replaced by  $\frac{1}{2}\pi i \delta''(p_0)$ . We carry out the  $p_0$  integration and transform the result to coordinate space, where the final

integration is carried out straightforwardly. Doubling the complete result for an equal contribution from  $[\text{OV}]_2$ , we find

$$2\Delta E([\text{VO}]_2; (\mathbf{p}-\mathbf{r})^2(\mathbf{p}'^2-\mathbf{p}\cdot\mathbf{p}')) = E_F \frac{\gamma^2}{m_e m_\mu} \left[ \ln \frac{m_r}{2\gamma} + \frac{5}{2} + C(E', E'') \right], \quad (4.2)$$

where some terms of higher order in  $\alpha$  have been neglected and we introduce

$$C(m_e, m_\mu) = \frac{m_\mu \ln \frac{m_e}{m_r} - m_e \ln \frac{m_\mu}{m_r}}{m_\mu - m_e} = \begin{cases} (\ln 2 - 1) & \text{for } m_\mu \rightarrow m_e \\ O[(m_e/m_\mu) \ln(m_\mu/m_e)] & \text{for } m_\mu \gg m_e. \end{cases}$$

For muonium, we may neglect  $C$ ; for positronium, our result is complete to this order in  $\alpha$ .

(ii)  $(\mathbf{p}-\mathbf{r})^2 \mathbf{p}'\cdot\mathbf{r}$ . This is simply treated. After using (3.18a), we find that the first term vanishes by symmetry ( $\mathbf{r} \leftrightarrow -\mathbf{r}$ ). The second term may be treated using the steps in (3.19). The final integral is easily performed by transforming to coordinate space with the result

$$2\Delta E([\text{VO}]_2; (\mathbf{p}-\mathbf{r})^2 \mathbf{p}'\cdot\mathbf{r}) = E_F \frac{\gamma^2}{m_e m_\mu} \left(-\frac{1}{2}\right). \quad (4.3)$$

(iii)  $-\mathbf{p}\cdot\mathbf{r}(\mathbf{p}-\mathbf{r})^2$ . The treatment of this term is similar to that of the previous ones. Using (3.18a), we find that the first term vanishes by symmetry ( $\mathbf{r} \leftrightarrow -\mathbf{r}$ ). The effect is to replace  $(\mathbf{p}-\mathbf{r})^2$  by  $p_0^2$ . Next we decouple the

$\mathbf{p}'$  integration using an expression similar to (3.18b); the decoupling correction is negligible. At this stage, the necessary integral is found in the tables  $[K_{13}(\mathbf{p}\cdot\mathbf{p}')]$ , so the result is

$$2\Delta E([\text{VO}]_2; -\mathbf{p}\cdot\mathbf{r}(\mathbf{p}-\mathbf{r})^2) = E_F \frac{\gamma^2}{m_e m_\mu} \left[ \ln \frac{m_r}{2\gamma} + C - 1 \right]. \quad (4.4)$$

(iv)  $(\mathbf{p}-\mathbf{r})\cdot(\mathbf{p}'-\mathbf{r})$ . By symmetry, the factor  $\mathbf{p}$  may be dropped. For the term  $\mathbf{p}'\cdot\mathbf{r}$  the calculation is like that for (4.3): it is twice as large and opposite in sign. With the  $\mathbf{r}^2$  term, we may decouple  $\mathbf{p}'$  using (3.18b) (with a relabeling). The integrals are found in the tables  $[K_{13}(\mathbf{p}'^2)]$ , with a relabeling. The complete result is

$$2\Delta E([\text{VO}]_2; (\mathbf{p}-\mathbf{r})\cdot(\mathbf{p}'-\mathbf{r})) = E_F \frac{\gamma^2}{m_e m_\mu} \left[ -4 \ln \frac{m_r}{2\gamma} + 2 - 4C \right]. \quad (4.5)$$

(v)  $p_0(\mathbf{p}'-\mathbf{r})^2$ . The  $-2\mathbf{p}'\cdot\mathbf{r}$  term is negligible ( $\approx \alpha^7 m_e^3/m_\mu^2$ ). To work out the  $\mathbf{p}'^2$  and  $\mathbf{r}^2$  terms, we decouple one of the wave functions using (3.18b), the second term of which yields a higher-order contribution. The  $\mathbf{p}'^2$  and  $\mathbf{r}^2$  terms give equal contributions, which may be looked up in the tables  $[K_7(\mathbf{p}'^2)]$ . The result is

$$2\Delta E([\text{VO}]_2; p_0(\mathbf{p}'-\mathbf{r})^2) = E_F \frac{\gamma^2}{m_e m_\mu}. \quad (4.6)$$

Including (3.20), we find that the total contribution from  $[\text{OV}]$  and  $[\text{VO}]$  is

$$2\Delta E([\text{VO}] + [\text{OV}]) = E_F \left[ -\frac{6\alpha}{\pi} \frac{m_e m_\mu}{m_\mu^2 - m_e^2} \ln \frac{m_\mu}{m_e} + \frac{\gamma^2}{m_e m_\mu} \left[ -2 \left[ \ln \frac{m_r}{2\gamma} + C \right] + 6 \right] \right]. \quad (4.7)$$

## 2. $[\text{VOO}]$ contribution

In Appendix B, we have analyzed the product of electron and muon factors and subtracted terms which are already taken into account in  $\text{V}$  and  $[\text{VO}]$ . The remaining terms are analyzed here.

We start with an expression similar to (3.16)

$$\Delta E([\text{VOO}]) = -(4\pi\alpha)^3 \frac{\frac{2}{3} \langle \boldsymbol{\sigma}_e \cdot \boldsymbol{\sigma}_\mu \rangle}{4E(m_\mu^2 - m_e^2)} \int \frac{d^3 p'' d^4 p' d^4 p d^3 r}{-(2\pi)^{14}} \frac{\phi_{\text{nr}}^\dagger(\mathbf{p}'') \phi_{\text{nr}}(\mathbf{r})}{D_e(p)} \times \frac{1}{[(p'' - p')^2 + i\epsilon][(p' - p)^2 + i\epsilon][(p - r)^2 + i\epsilon]} (\mathbf{J}_e - \mathbf{J}_\mu + \mathbf{M}), \quad (4.8)$$

where

$$\mathbf{J}_e = \frac{-2\pi i \delta(p_0)(\mathbf{p}-\mathbf{r})^2}{D_e(p')} \left[ 2m_\mu(2m_e + p'_0) + \frac{4m_\mu m_e (\mathbf{p}' - \mathbf{p}'') \cdot (\mathbf{p}' - \mathbf{p})}{(p'_0 + i\epsilon)^2} \right] = \mathbf{J}'_e + \mathbf{J}''_e,$$

with a similar expression for  $J_\mu$ , and

$$M = \frac{m_\mu}{D_e(p')} \left[ (\mathbf{p}-\mathbf{r})^2 2\mathbf{p}\cdot\mathbf{p} \left[ \frac{-4\pi i\delta(p_0-p'_0)m_e}{(p_0+i\epsilon)^2} + \frac{2\pi i\delta(p_0)-2\pi i\delta(p_0-p'_0)}{p'_0+i\epsilon} \right] \right. \\ \left. + (\mathbf{p}-\mathbf{r})\cdot(\mathbf{p}'-\mathbf{r}) \left[ (2m_e+p'_0)4\pi i\delta(p_0-p'_0) + \frac{2\mathbf{p}\cdot\mathbf{p}'[2\pi i\delta(p'_0)-2\pi i\delta(p_0-p'_0)]}{p_0+i\epsilon} \right] \right. \\ \left. + (\mathbf{p}'-\mathbf{r})^2 p_0 4\pi i\delta(p_0-p'_0) \right].$$

The  $J_\beta$  terms in (4.8) are symmetric in the two leptons. This is important because they yield a  $\ln\alpha$  contribution from the low-momentum region, and we wish to obtain the correct mass-symmetric coefficient for such logarithms. The  $M$  term emphasizes momenta which are relativistic for the electron, but nonrelativistic for the muon. In obtaining it, we have therefore made an expansion in powers of  $m_e/m_\mu$  and retained only the leading term. Thus contributions from  $M$  are not valid for positronium, while those from  $J_\beta$  are. At the present, we have little hope of making a complete analytic calculation for positronium.

Now we proceed to the evaluation of (4.8), starting with the  $J_\beta$  terms. The factor of  $(\mathbf{p}-\mathbf{r})^2$ , together with  $\delta(p_0)$ , leads to a decoupling of the  $\mathbf{r}$  integration. With the  $J'_\beta$  term, the  $\mathbf{p}''$  integration is also decoupled, following the strategy embodied in (3.18b). By using (3.19), one finds that the correction terms to the decoupling are negligible. The integrals for the  $J'_\beta$  terms are then easily expressed in terms of  $K_{12}(\mathbf{p}^2+\gamma^2)$  and  $K_8(\mathbf{p}^2+\gamma^2)$ . The result is

$$2\Delta E([\text{VOO}], J') = E_F \frac{\gamma^2}{m_e m_\mu} \left[ -2 \left[ \ln \frac{m_r}{2\gamma} + C \right] + \frac{1}{2} \right]. \tag{4.9a}$$

The  $J''_\beta$  terms yield one of the more complicated integrals which we encounter. It is a three-loop integral of a particularly delicate nature. The numerator momentum dependence is very important because it prevents a divergence at small momenta after the  $p'_0$  integration has been carried out. Our procedure for evaluating the integral is rather brute force in nature, but it works. We first use (3.18b) to decouple the  $\mathbf{p}''$  integration. The resulting integral arising from the first term of (3.18b) is given in the tables as  $K_{15}((\mathbf{p}^2+\gamma^2)(\mathbf{p}'-\mathbf{p})\cdot\mathbf{p}')$ ; note that in this case the  $\mathbf{p}''$  term vanishes by symmetry. The second (decoupling) term arises from the low-momentum region, so we may treat the lepton denominator as in the first step of (3.19). Now the factor of  $1/(p'_0+i\epsilon)^3$  may be replaced by the second derivative of  $\delta(p'_0)$ , using the fact that the rest of the integrand is even in  $p'_0$ . The subsequent integral may be evaluated straightforwardly, but tediously, by transforming it to coordinate space. The final result is

$$2\Delta E([\text{VOO}], J'') = E_F \frac{\gamma^2}{m_e m_\mu} \left[ -2 \left[ \ln \frac{m_r}{2\gamma} + C \right] \right]. \tag{4.9b}$$

The contribution from  $M$  may be evaluated rather straightforwardly by first noting that the  $\mathbf{p}''$  and  $\mathbf{r}$  integrations may be decoupled with negligible correction. This is consistent with Appendix B, in which wavefunction momenta dependence in the kernel has already been neglected for this term. For the convenience of the dedicated reader, we will simply cite the integrals which are used for the various terms. For the first of the two terms with a factor  $(\mathbf{p}-\mathbf{r})^2 (\approx \mathbf{p}^2)$ , we use  $K_{14}(\mathbf{p}^2\mathbf{p}\cdot\mathbf{p}')$ ; for the second we use  $K_5(\mathbf{p}^2\mathbf{p}\cdot\mathbf{p}')$ . For the first term with the factor  $(\mathbf{p}-\mathbf{r})\cdot(\mathbf{p}'-\mathbf{r}) (\approx \mathbf{p}'\cdot\mathbf{p})$ , we use  $K_{11}(\mathbf{p}\cdot\mathbf{p}')$  and  $K_9(\mathbf{p}\cdot\mathbf{p}')$ ; for the second we use  $K_6((\mathbf{p}\cdot\mathbf{p}')^2)$ . In the final term we make use of  $K_9(\mathbf{p}^2)$ . When added together, these yield

$$2\Delta E([\text{VOO}], M) = E_F \frac{\gamma^2}{m_e m_\mu} (-12 \ln 2 + 2\frac{1}{2}). \tag{4.9c}$$

The total result is then

$$\Delta E([\text{VOO}]+[\text{OOV}]) = E_F \frac{\gamma^2}{m_e m_\mu} \left[ -4 \left[ \ln \frac{m_r}{2\gamma} + C \right] - 12 \ln 2 + 3 \right]. \tag{4.10}$$

### 3. [OVO] contribution

In Appendix B, the integrand of OVO is analyzed and the appropriate V, [OV], and [VO] terms are subtracted. The result is extremely simple in comparison to our previous work. All contributions are relativistic for the electron. The wave functions may be decoupled with negligible corrections, and the integral which must be evaluated turns out to be



$$\begin{aligned}
\Delta E([\text{OVO}]) = & -(4\pi\alpha)^3 \frac{\frac{2}{3} \langle \boldsymbol{\sigma}_e \cdot \boldsymbol{\sigma}_\mu \rangle}{4m_\mu^2} \frac{\gamma^3}{\pi} \\
& \times \int \frac{d^4p d^4r}{(4\pi)^8} \frac{2\mathbf{p} \cdot \mathbf{r}}{D_e(p)D_e(r)} \frac{1}{(p^2 - \gamma^2 + i\epsilon)[(p-r)^2 - \gamma^2 + i\epsilon](r^2 - \gamma^2 + i\epsilon)} \\
& \times \left[ (\mathbf{p}-\mathbf{r})^2 \frac{4\pi i \delta(r_0 - p_0) m_e}{(r_0 + i\epsilon)^2} - \mathbf{r} \cdot (\mathbf{p}-\mathbf{r}) \frac{2\pi i \delta(r_0) - 2\pi i \delta(p_0 - r_0)}{p_0 + i\epsilon} \right. \\
& \left. + \mathbf{p} \cdot (\mathbf{p}-\mathbf{r}) \frac{2\pi i \delta(p_0) - 2\pi i \delta(p_0 - r_0)}{r_0 + i\epsilon} \right]. \tag{4.11}
\end{aligned}$$

In the first term of (4.11), the combination of the  $\delta$  function and the factor  $(\mathbf{p}-\mathbf{r})^2$  causes the  $\mathbf{r}$  and  $\mathbf{p}$  angular integrations to vanish. For the remaining terms, the necessary integral is  $K_5[\mathbf{p} \cdot \mathbf{p}' \cdot (\mathbf{p}-\mathbf{p}')]$  and the result is

$$\Delta E([\text{OVO}]) = E_F \frac{\gamma^2}{m_e m_\mu} \left( \frac{1}{4} \right). \tag{4.12}$$

#### 4. Summary of the one-V contribution

Adding (3.15b), (4.7), (4.10), and (4.12), we find for the complete one-V contribution

$$\Delta E(*\text{V}*) = E_F \left[ 1 + \frac{3}{2} \alpha^2 - \frac{6\alpha}{\pi} \frac{m_e m_\mu}{m_\mu^2 - m_e^2} \ln \frac{m_\mu}{m_e} + \frac{\gamma^2}{m_e m_\mu} \left[ -6 \left[ \ln \frac{m_r}{2\gamma} + C \right] - 12 \ln 2 + 10 \frac{3}{4} \right] \right]. \tag{4.13}$$

Recall that the nonlogarithmic part of the last term is not reliable for positronium, although some of its pieces are.

### B. Contributions involving two V's

The general approach to the calculation of the two-V terms is similar to that of the one-V terms, and the amount of effort is of the same order of magnitude. These terms include a leading one-loop piece, already worked out in Sec. III.E. In this section, other terms of the current order of interest are considered. As before, the basic algebra for the various terms is carried out in Appendix B; and we study the resulting integrals here. The pattern of the discussion for each distinct contribution is the same: presentation of the integrand factor, description of the way in which the integration is performed, and tabulation of the result to the order of interest.

#### 1. Remainder from [VV]

The integrand for VV is analyzed in Appendix B Sec. 2.a, but is not written out there explicitly. The sources of various terms, omitting photon and wave functions factors, is as follows. The product of Eqs. (B23) and (B24) yields three contributions corresponding to the three terms of (B23). The first of these, the one-loop contribution, is worked out in Sec. III.E. The other terms are broken down further and calculated here. They have the structure

$$\Delta E([\text{VV}]) = (4\pi\alpha)^2 \frac{\frac{2}{3} \langle \boldsymbol{\sigma}_e \cdot \boldsymbol{\sigma}_\mu \rangle}{m_\mu^2 - m_e^2} \int \frac{d^3p' d^4p d^3r}{(2\pi)^{10} i} \frac{\phi_{nr}^\dagger(\mathbf{p}') \phi_{nr}(\mathbf{r})}{[(p-p')^2 + i\epsilon][(p-r)^2 + i\epsilon]} [I_e([\text{VV}]) - I_\mu([\text{VV}])]. \tag{4.14}$$

(i) *Second term of [VV] (label: [VV]:#2).* The part of  $I_e$  corresponding to the second term of (B23) is

$$I_e([\text{VV}]:\#2) = \frac{-(2p_0^2 - \mathbf{p}^2 - \gamma^2)(3\gamma^2 + \mathbf{p}' \cdot \mathbf{p} + \mathbf{p}' \cdot \mathbf{r} + \mathbf{p}' \cdot \mathbf{r})}{8m_e D_e(p)} \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right].$$

The combination  $3\gamma^2 + \mathbf{p}' \cdot \mathbf{r}$  in the second factor contributes only with  $\delta(p_0)$  in the third factor; the resulting integrals are easy. In the remaining terms, we may decouple the  $\mathbf{r}$  or the  $\mathbf{p}'$  integrations using (3.18b) (only the first term contributes). The decoupling corrections are either zero [with  $\delta(p_0)$ ] or negligible [with  $1/(p_0 + i\epsilon)$ ]. The necessary integrals are given by  $K_7(\mathbf{p}' \cdot \mathbf{p})$  and  $K_1[\mathbf{p}' \cdot \mathbf{p}(p^2 + \gamma^2)]$ , and the complete result is

$$\Delta E([VV];\#2) = E_F \frac{\gamma^2}{m_e m_\mu} \left[ - \left[ \ln \frac{m_r}{2\gamma} + C \right] - \frac{1}{8} \right]. \tag{4.15}$$

Third term of [VV] (labels given later). This term has one of the most complicated matrix structures we encounter. It contains the product

$$C_{ij}^e D_{ij}^\mu = (2m_e + \alpha_e \cdot \mathbf{p}') \alpha_{ei} (E' + \beta_e m_e + \alpha_e \cdot \mathbf{p}) \alpha_{ej} (2m_e + \alpha_e \cdot \mathbf{r}) / (2m_e) \otimes (\alpha_\mu \cdot \mathbf{p}' \alpha_{\mu i} + \alpha_{\mu i} \alpha_\mu \cdot \mathbf{p}) (\alpha_\mu \cdot \mathbf{p} \alpha_{\mu j} + \alpha_{\mu j} \alpha_\mu \cdot \mathbf{r}). \tag{4.16a}$$

As in Sec. II.B, it is convenient to decompose the factors of  $D_{ij}$  into convection and spin parts:

$$\begin{aligned} -(\alpha_\mu \cdot \mathbf{p}' \alpha_{\mu i} + \alpha_{\mu i} \alpha_\mu \cdot \mathbf{p}) &= -(\mathbf{p}' + \mathbf{p})_i - i[\sigma_\mu \times (\mathbf{p}' - \mathbf{p})]_i, \\ -(\alpha_\mu \cdot \mathbf{p} \alpha_{\mu j} + \alpha_{\mu j} \alpha_\mu \cdot \mathbf{r}) &= -(\mathbf{p} + \mathbf{r})_j - i[\sigma_\mu \times (\mathbf{p} - \mathbf{r})]_j. \end{aligned} \tag{4.16b}$$

Clearly, the combination of two convection factors does not contribute to the hfs, so we consider the other possible combinations. The product of a convection factor from the muon with an  $\alpha$  matrix from the electron is rearranged in the same manner as in the steps leading to (2.23c):

$$\begin{aligned} -\alpha_e \cdot (\mathbf{p}' + \mathbf{p}) &= [E' - H_e(\mathbf{p}')] + [E' - H_e(\mathbf{p})] \\ &\quad - 2(E' - \beta_e m_e). \end{aligned} \tag{4.16c}$$

We label the various contributions which arise from this expression by the terms on the rhs.

(ii)  $-2(E' - \beta_e m_e)$ . This contribution need not be evaluated. With  $-2\pi i \delta(p_0)$ , it produces the  $V_c'$  term necessary for the compensation of the term  $(VO)_1$  of Appendix B Sec. 1.d; and with  $2/(p_0 + i\epsilon)$ , it gives a completely negligible contribution.

(iii)  $E' - H_e(\mathbf{p}')$ . Using the structure of the electron factor, we find the expression

$$\begin{aligned} I_e([VV]; E' - H_e(\mathbf{p}')) &= \frac{-(\mathbf{p}'^2 + \gamma^2)(\mathbf{p} - \mathbf{r})^2}{8m_e D_e(p)} \\ &\quad \times \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right]. \end{aligned} \tag{4.17a}$$

We use (3.18a) to rearrange the expression. In the second term of the right-hand side of (3.18a), we then use (3.18b), keeping only the first term (the decoupling correction is negligible). When the terms are recombined, the result is equivalent to having replaced  $(\mathbf{p} - \mathbf{r})^2$  by  $\mathbf{p}^2 + \gamma^2$  in the numerator and denominator of the integrand. The com-

plete result, obtained from  $K_1[(\mathbf{p}^2 + \gamma^2)(\mathbf{p}'^2 + \gamma^2)]$ , is doubled to take into account the symmetric term  $E' - H_e(\mathbf{r})$ :

$$\begin{aligned} 2\Delta E([VV]; E' - H_e(\mathbf{p}')) &= E_F \frac{\gamma^2}{m_e m_\mu} \\ &\quad \times \left[ 2 \left[ \ln \frac{m_r}{2\gamma} + C \right] - \frac{1}{2} \right]. \end{aligned} \tag{4.17b}$$

$E' - H_e(\mathbf{p})$ : The numerator is found to have the structure

$$-(\mathbf{p}^2 + \gamma^2) \sigma_e \times (\mathbf{p}' - \mathbf{r}) \cdot \sigma_\mu \times (\mathbf{p} - \mathbf{r}).$$

The similar term that arises from the other choice of spin and convection on the muon side modifies this to

$$-\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle (\mathbf{p}^2 + \gamma^2)(\mathbf{p}' - \mathbf{r})^2,$$

and we find the factor in the integrand

$$\begin{aligned} I_e([VV]; E' - H_e(\mathbf{p})) &= \frac{-(\mathbf{p}^2 + \gamma^2)(\mathbf{p}' - \mathbf{r})^2}{8m_e D_e(p)} \\ &\quad \times \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right]. \end{aligned} \tag{4.18a}$$

The  $\mathbf{p}'^2$  and  $\mathbf{r}^2$  terms in the second factor yield identical contributions. After we decouple one of the wave functions, they can be expressed in terms of  $K_1[\mathbf{p}'^2(\mathbf{p}^2 + \gamma^2)]$ . For the  $\mathbf{p}' \cdot \mathbf{r}$  term only  $\delta(p_0)$  contributes. The complete result is

$$\begin{aligned} \Delta E([VV]; E' - H_e(\mathbf{p})) &= E_F \frac{\gamma^2}{m_e m_\mu} \\ &\quad \times \left[ 2 \left[ \ln \frac{m_r}{2\gamma} + C \right] - \frac{3}{2} \right]. \end{aligned} \tag{4.18b}$$

(iv) *Spin-spin*. The contribution to (4.16a) is

$$\sigma_e \times (\mathbf{p}' - \mathbf{p}) \cdot \sigma_\mu \times (\mathbf{p}' - \mathbf{p}) \sigma_e \times (\mathbf{p} - \mathbf{r}) \cdot \sigma_\mu \times (\mathbf{p} - \mathbf{r}) + (\mathbf{p}^2 + \gamma^2) \sigma_e \cdot \sigma_\mu \times (\mathbf{p}' - \mathbf{p}) \sigma_e \cdot \sigma_\mu \times (\mathbf{p} - \mathbf{r}). \tag{4.19a}$$

In deriving this expression, it is useful to start with the second form of  $C_{ij}$  given in Eq. (B23a). Note also that we have dropped terms involving  $\sigma_\mu \cdot (\mathbf{p}' \times \mathbf{p})$  since they vanish when one carries out the  $\mathbf{p}'$  integration. The combination  $\mathbf{p}^2 + \gamma^2$  is helpful for avoiding some complicated integrals (yielding spurious  $\pi^2$  terms) which would arise if the two pieces were separated. This type of simplification is not obvious, and in earlier versions of our analysis these complications did occur.

The expression (4.19a) may be "simplified" using brute-force application of the rules for products of  $\sigma$  matrices together with spherical averaging of the integrand. We find

$$\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle \left\{ -\frac{3}{2} (\mathbf{p}' - \mathbf{p})^2 (\mathbf{p} - \mathbf{r})^2 + (\mathbf{p}^2 + \gamma^2) (\mathbf{p} - \mathbf{r}) \cdot (\mathbf{p} - \mathbf{p}') + \frac{1}{2} [(\mathbf{p}' - \mathbf{p}) \cdot (\mathbf{p} - \mathbf{r})]^2 \right\}.$$

This is now rearranged into terms that are convenient for computation to give a contribution to the integrand

$$\begin{aligned} I_e([\mathbf{V}\mathbf{V}]; \text{spin-spin}) = & \left( -\frac{3}{2} [(\mathbf{p}' - \mathbf{p})^2 - \mathbf{p}^2 - \gamma^2] [(\mathbf{p} - \mathbf{r})^2 - \mathbf{p}^2 - \gamma^2] \right. \\ & - \frac{3}{2} (\mathbf{p}^2 + \gamma^2) [(\mathbf{p}' - \mathbf{p})^2 + (\mathbf{p} - \mathbf{r})^2 - 2\mathbf{p}^2] + (\mathbf{p}^2 + \gamma^2) [\mathbf{p}' \cdot \mathbf{r} - 2\mathbf{p} \cdot (\mathbf{p}' + \mathbf{r})] \\ & + \frac{1}{2} (\mathbf{p} \cdot \mathbf{r})^2 + \frac{1}{2} (\mathbf{p} \cdot \mathbf{p}')^2 + \frac{1}{2} \{ [(\mathbf{p}' - \mathbf{p}) \cdot (\mathbf{p} - \mathbf{r})]^2 - [\mathbf{p} \cdot (\mathbf{p}' - \mathbf{p})]^2 - [\mathbf{p} \cdot (\mathbf{p} - \mathbf{r})]^2 + \mathbf{p}^4 \} \\ & \left. + \gamma^2 [\mathbf{p}^2 + \mathbf{p} \cdot (\mathbf{p}' + \mathbf{r}) + \frac{3}{2} \gamma^2] \right) \frac{1}{8m_e D_e(p)} \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right]. \end{aligned} \quad (4.19b)$$

Any term in this expression which contains both  $\mathbf{p}'$  and  $\mathbf{r}$  or factors of  $\gamma^2$  can contribute to the order of interest only in combination with  $\delta(p_0)$ . Thus the first term gives zero when the wave function integrations are carried out. In the second term we can always decouple one of the wave functions and work out the integral in terms of  $K_1[(\mathbf{p}^2 + \gamma^2)(\mathbf{p}'^2 - 2\mathbf{p}' \cdot \mathbf{p})]$ ; because of its structure, it contributes no  $\ln \alpha$ . The piece of the third term containing  $\mathbf{p}' \cdot \mathbf{r}$  is easily worked out. Again the combination  $\mathbf{p}^2 + \gamma^2$  makes the calculation simple; without it, the separate integrals would be more complicated and they would yield spurious  $\pi^2$  contributions. It is, unfortunately, very easy to arrange the algebra in such a way that these simplifications are overlooked. The other parts of the third term can be evaluated by decoupling one of the wave functions and using  $K_1[(\mathbf{p}^2 + \gamma^2)\mathbf{p}' \cdot \mathbf{p}]$ . The fourth and fifth terms are evaluated by similar techniques in terms of  $K_1[(\mathbf{p}' \cdot \mathbf{p})^2]$ . The sixth term requires quite an elaborate analysis in coordinate space in which the tensor structure of the resulting derivative operators is decomposed into  $S$  and  $D$  wave parts (see Appendix C). The final term can be evaluated in terms of  $K_1[\gamma^2(\mathbf{p}'^2 + 2\mathbf{p}' \cdot \mathbf{p} + \frac{3}{2}\gamma^2)]$ . The net result is

$$\Delta E([\mathbf{V}\mathbf{V}]; \text{spin-spin}) = E_F \frac{\gamma^2}{m_e m_\mu} \left[ \frac{3}{2} \left( \ln \frac{m_r}{2\gamma} + C \right) - \frac{3}{4} \right]. \quad (4.19c)$$

The complete result from  $[\mathbf{V}\mathbf{V}]$ , including the one-loop contribution (3.22b), is

$$\Delta E([\mathbf{V}\mathbf{V}]) = E_F \left\{ \frac{3\alpha}{\pi} \frac{m_e m_\mu}{m_\mu^2 - m_e^2} \ln \frac{m_\mu}{m_e} + \frac{\gamma^2}{m_\mu m_e} \left[ \frac{9}{2} \left( \ln \frac{m_r}{2\gamma} + C \right) - 7\frac{3}{8} \right] \right\}. \quad (4.20)$$

## 2. $[\mathbf{V}\mathbf{V}\mathbf{O}]$ contribution

Most of  $\mathbf{V}\mathbf{V}\mathbf{O}$  is subtracted away by terms from  $[\mathbf{V}\mathbf{V}]$ ; wave functions have been decoupled using the first term of (3.18b), with negligible remainder. The expression to be evaluated is

$$\begin{aligned} \Delta E([\mathbf{V}\mathbf{V}\mathbf{O}]) = & (4\pi\alpha)^3 \frac{\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle \gamma^3}{4E^2\pi} \\ & \times \int \frac{d^4 p' d^4 p}{(2\pi)^8} \frac{1}{D_e(p') D_e(p)} \frac{1}{(p'^2 - \gamma^2 + i\epsilon) [(p' - p)^2 + i\epsilon] (p^2 - \gamma^2 + i\epsilon)} \\ & \times \left[ 2[(\mathbf{p}' \cdot \mathbf{p}')^2 - \mathbf{p}'^2 \mathbf{p} \cdot \mathbf{p}' - \mathbf{p}^2 \mathbf{p}' \cdot \mathbf{p}' + \mathbf{p}'^2 \mathbf{p}^2] \left[ \frac{-2\pi i \delta(p'_0) + 2\pi i \delta(p'_0 - p_0)}{p_0 + i\epsilon} \right] \right. \\ & \left. + 2(\mathbf{p}'^2 + \mathbf{p}' \cdot \mathbf{p}) \mathbf{p}^2 \left[ \frac{-2\pi i \delta(p_0)}{p'_0 + i\epsilon} + \frac{2\pi i \delta(p'_0)}{p_0 + i\epsilon} \right] + 2(\mathbf{p}'^2 - 2\mathbf{p}' \cdot \mathbf{p}) 2\pi i \delta(p'_0) p_0 \right]. \end{aligned} \quad (4.21a)$$

The three terms in the large parentheses of (4.21a) are given (in succession) by the integrals  $2K_6[(\mathbf{p}' \cdot \mathbf{p}')^2 - \mathbf{p}'^2 \mathbf{p} \cdot \mathbf{p}' - \mathbf{p}^2 \mathbf{p}' \cdot \mathbf{p}' + \mathbf{p}'^2 \mathbf{p}^2]$ ,  $2K_4(\mathbf{p}'^2 \mathbf{p}^2 + \mathbf{p}^2 \mathbf{p}' \cdot \mathbf{p}')$ , and  $-2K_7(\mathbf{p}'^2 - 2\mathbf{p}' \cdot \mathbf{p})$ . The total contribution is

$$\Delta E([\mathbf{V}\mathbf{V}\mathbf{O}]) = 0. \quad (4.21b)$$

3. [VOV] contribution

This contribution does not involve any subtractions of previously calculated terms. As in the earlier cases, the algebraic analysis of the integrand is given in Appendix B. In this case, we do not present an expression which is symmetric in the two particles, but assure the reader that the contribution containing  $\ln\alpha$  has the correct mass-symmetric coefficient. It is possible to arrange the various terms so that the argument of the logarithm is mass symmetric, also, as in (4.2), but we did not choose to follow such a procedure, since it seems rather artificial in the present instance.

The integral for [VOV] is

$$\Delta E([\text{VOV}]) = (4\pi\alpha)^3 \int \frac{d^3p'' d^4p' d^4p d^3r}{-(2\pi)^{14}} \frac{\psi^\dagger(\mathbf{p}'') EF([\text{VOV}]) \psi(\mathbf{r})}{D_e(p') D_e(p)} \times \frac{1}{[(p''-p')^2+i\epsilon][(p'-p^2)+i\epsilon][(p-r)^2+i\epsilon]} MF([\text{VOV}]), \tag{4.22}$$

where

$$EF([\text{VOV}]) = \alpha_{ei}[E'+p'_0+H_e(\mathbf{p}')][E'+p_0+H_e(\mathbf{p})]\alpha_{ej}$$

and

$$MF([\text{VOV}]) = \frac{(\alpha_\mu \cdot \mathbf{p}'' \alpha_{\mu i} + \alpha_{\mu i} \alpha_\mu \cdot \mathbf{p}')(\alpha_\mu \cdot \mathbf{p} \alpha_{\mu j} + \alpha_{\mu j} \alpha_\mu \cdot \mathbf{r})}{4E^2} \left[ (-2\pi i)^2 \delta(p_0) \delta(p'_0) + \frac{2\pi i \delta(p_0)}{p'_0 + i\epsilon} + \frac{2\pi i \delta(p'_0)}{p_0 + i\epsilon} \right] - \frac{\alpha_\mu \cdot (\mathbf{p}' - \mathbf{p}) \alpha_{\mu i} \alpha_\mu \cdot \mathbf{p} \alpha_{\mu j} + p^2 \alpha_{\mu i} \alpha_{\mu j}}{4m_\mu^2} \left[ \frac{-2\pi i \delta(p_0) + 2\pi i \delta(p'_0 - p_0)}{p'_0 + i\epsilon} \right] + \frac{\alpha_\mu \cdot (\mathbf{p} - \mathbf{p}') \alpha_{\mu j} \alpha_\mu \cdot \mathbf{p}' \alpha_{\mu i} + p'^2 \alpha_{\mu j} \alpha_{\mu i}}{4m_\mu^2} \left[ \frac{-2\pi i \delta(p'_0) + 2\pi i \delta(p'_0 - p_0)}{p_0 + i\epsilon} \right].$$

Analysis of this integral leads to a proliferation of terms. However, all the techniques for handling them have now been developed, so in the following discussions we present only the main strategy and leave some of the special details to Appendix C. The first (and most important) term in  $MF$  is handled with the same breakdowns used in (4.16b) and (4.16c), but with relabeled arguments, of course. We start with the contribution involving one convection and one spin factor in the muon line.

(i)  $E' - H_e(\mathbf{p}'')$ . Acting on the wave function, this expression can be replaced by  $V_c$ . A contribution of the order of interest can now be obtained only in combination with *both* accompanying  $\delta$  functions. But then we see that this is just the contribution we need to cancel the first term of (2.27), as was mentioned there. Taking into account a contribution from the change of gauge in Sec. III.C, we find that all of (2.27) has now been canceled.

(ii)  $-2(E' - \beta_e m_e)$ . In a similar manner, this produces a factor of  $V'_c$ , leading to the cancellation of the term  $(\text{VOO})_1$  from Appendix B Sec. 1.d.

(iii)  $E' - H_e(\mathbf{p}')$ . We rearrange this to

$$E' - H_e(\mathbf{p}') = [E' + p'_0 - H_e(\mathbf{p}')] - p'_0. \tag{4.23a}$$

The first term gives a contribution which may be identified with a previously calculated contribution in [VV]. To see this, we note that the denominator  $D_e(p')$  is canceled out. Then the symmetry of the integral permits us to replace  $1/(p'_0 + i\epsilon)$  by  $-i\pi\delta(p'_0)$ . Now we carry out the  $\mathbf{p}''$  integration using (3.17b). At this stage, the expression is identical to the one which results from (4.17a), ex-

cept that it is half as large and the factor

$$\frac{1}{E'' - E'} \left[ \frac{E''}{D_e(p)} - \frac{E'}{D_\mu(p)} \right]$$

has been replaced by

$$\frac{1}{D_e(p)}.$$

The effect of this change of factors is to modify the argument of the logarithm by an amount which gives a negligible contribution for muonium.

The second term of (4.23a) gives a contribution which can also be expressed in terms of previously worked out contributions. To the order of interest, the electron numerator operator which occurs between nonrelativistic wave functions is  $p'_0(2m_e + p'_0)\alpha_e \cdot (\mathbf{p} - \mathbf{r})\alpha_{ej}$ . The resulting integrand turns out to be  $-\frac{1}{2}$  of that given by the  $J'$  piece of (4.8) (aside from terms of the type just discussed, which modify the argument of the  $\ln$ ). Thus the total result from  $E' - H_e(\mathbf{p}')$  is

$$2\Delta E([\text{VOV}]; E' - H_e(\mathbf{p}')) = E_F \frac{\gamma^2}{m_\mu m_e} \left[ 2 \ln \frac{m_r}{2\gamma} - \frac{1}{2} \right]. \tag{4.23b}$$

(iv) *Spin-spin*. It is easy to see that, to the order of interest, only the spin-spin part of the electron factor contributes. We rearrange the resulting product as

$$\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle \left( -\frac{3}{2} (\mathbf{p}'' - \mathbf{p}')^2 (\mathbf{p} - \mathbf{r})^2 + \frac{1}{2} (\mathbf{p}' \cdot \mathbf{p})^2 + \frac{1}{2} \{ [(\mathbf{p}'' - \mathbf{p}') \cdot (\mathbf{p} - \mathbf{r})]^2 - (\mathbf{p}' \cdot \mathbf{p})^2 \} \right). \tag{4.24a}$$

With the first term, we decouple the wave functions using (3.18). The second term of (3.18b) gives a negligible contribution, and we find that the result is expressed in terms of  $K_1[(\mathbf{p}'^2 + \gamma^2)(\mathbf{p}^2 + \gamma^2)]$ . The second term is treated in the same manner, and the result is given by  $K_1[(\mathbf{p}' \cdot \mathbf{p})^2]$ . The third term contains factors of  $\mathbf{p}''$  and  $\mathbf{r}$ , so it contributes only with two  $\delta$  functions in (4.22). The resulting four-loop integral is worked out by splitting up the interactions into  $S$ -wave and  $D$ -wave parts (as in the similar term of [VV]; see Appendix C). The complete result is

$$\Delta E([\text{VOV}]; \text{spin-spin}) = E_F \frac{\gamma^2}{m_\mu m_e} \left[ \frac{5}{4} \ln \frac{m_e}{2\gamma} - \frac{1}{8} \right]. \tag{4.24b}$$

(v) *Remainder.* We lump all the remaining terms together, since they present no special problems, and describe briefly how they are worked out. They are arranged according to the number of spatial powers of momentum which occur. Those with four such powers lead to the integral  $K_6[(\mathbf{p}' \cdot \mathbf{p})^2 - 3\mathbf{p}'^2 \mathbf{p}^2 - 4\mathbf{p}'^2 \mathbf{p} \cdot \mathbf{p}']$  (not symmetrized with respect to  $\mathbf{p} \leftrightarrow \mathbf{p}'$ ). Those with two such

powers yield  $K_9[(\mathbf{p}' - \mathbf{p})^2]$ , and those with none yield  $-6K_{10}$ . The total result is

$$\Delta E([\text{VOV}]; \text{rem}) = E_F \frac{\gamma^2}{m_\mu m_e} (6 \ln 2 - 2). \tag{4.25}$$

The complete result for [VOV] is then

$$\Delta E([\text{VOV}]) = E_F \frac{\gamma^2}{m_\mu m_e} \left[ \frac{13}{4} \ln \frac{m_e}{2\gamma} + 6 \ln 2 - 2 \frac{5}{8} \right]. \tag{4.26}$$

4. Summary of the two-V contribution

Adding (4.20), (4.21b), and (4.26), we find

$$\Delta E(V * V) = E_F \left[ \frac{3\alpha}{\pi} \frac{m_e m_\mu}{m_\mu^2 - m_e^2} \ln \frac{m_\mu}{m_e} + \frac{\gamma^2}{m_\mu m_e} \left[ \frac{31}{4} \ln \frac{m_e}{2\gamma} + 6 \ln 2 - 10 \right] \right]. \tag{4.27}$$

C. The OOO-OO contribution

As we found in Appendix B, an expression which gives the coefficient of  $\ln \alpha$  correctly, but is otherwise not valid for positronium, is

$$\begin{aligned} \Delta E([\text{OOO}]) = & (4\pi\alpha)^3 \frac{\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle}{4E^2} \int \frac{d^3 p'' d^4 p' d^4 p d^3 r}{-(2\pi)^{14}} \frac{-\frac{1}{2} \mathbf{p}'^2 \mathbf{p}^2 + \frac{1}{2} (\mathbf{p}' \cdot \mathbf{p})^2}{D_e(p') D_e(p)} \\ & \times \frac{\phi_{nr}^\dagger(\mathbf{p}'') \phi_{nr}(\mathbf{r})}{[(p'' - p')^2 + i\epsilon][(p' - p)^2 + i\epsilon][(p - r)^2 + i\epsilon]} \\ & \times \left[ (-2\pi i)^2 \delta(p'_0) \delta(p_0) + \frac{4\pi i \delta(p'_0)}{p_0 + i\epsilon} + \frac{4\pi i \delta(p_0)}{p_0 + i\epsilon} - \frac{4\pi i \delta(p'_0 - p_0)}{p_0 + i\epsilon} \right]. \end{aligned} \tag{4.28}$$

We can decouple the wave function integrations using (3.18b), neglecting the decoupling corrections. The result is given by  $\frac{1}{2} K_1[-\mathbf{p}'^2 \mathbf{p}^2 + (\mathbf{p}' \cdot \mathbf{p})^2] + K_5[\mathbf{p}'^2 \mathbf{p}^2 - (\mathbf{p}' \cdot \mathbf{p})^2]$ , and we find

$$\Delta E([\text{OOO}]) = E_F \frac{\gamma^2}{m_e m_\mu} \left[ \frac{1}{4} \ln \frac{m_e}{2\gamma} - \frac{3}{8} \right]. \tag{4.29}$$

D. The VVV contribution

This contribution is given by the integral

$$\begin{aligned} \Delta E([\text{VVV}]) = & -(4\pi\alpha)^3 \frac{\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle}{4E^2} \int \frac{d^3 p'' d^4 p' d^4 p d^3 r}{-(2\pi)^{14}} \frac{\phi_{nr}^\dagger(\mathbf{p}'') \phi_{nr}(\mathbf{r})}{[(p'' - p')^2 + i\epsilon][(p' - p)^2 + i\epsilon][(p - r)^2 + i\epsilon]} \\ & \times [-2\pi i \delta(p_0) 6p'_0 \mathbf{p}^2 - 2\pi i \delta(p'_0) 6p_0 \mathbf{p}'^2 + 2\pi i \delta(p_0 - p'_0) 2p_0 (\mathbf{p} - \mathbf{p}')^2]. \end{aligned} \tag{4.30}$$

We may decouple the wave function integrations and use the integrals  $K_7(\mathbf{p}'^2)$ ,  $K_8(\mathbf{p}^2)$ , and  $K_9[(\mathbf{p} - \mathbf{p}')^2]$  to find

$$\Delta E([\text{VVV}]) = E_F \frac{\gamma^2}{m_e m_\mu} \left( \frac{5}{4} \right). \tag{4.31}$$

V. SECOND-ORDER PERTURBATION THEORY

In this section we discuss contributions to the energy shift which are second order in the perturbation kernels—that is, contributions from the second, third, and

fourth terms of (2.13b). If we are to obtain a contribution of the order of interest [ $O(\alpha^6)$ ] from the sum over states, matrix elements of  $\hat{K}$  must be  $O(\alpha^4)$ . This follows from the fact that the energy denominators are  $O(\alpha^2)$ . The kernels satisfying this criterion are the spin and convection parts of the one-transverse photon exchange [ $\hat{K}(\text{spin})$  is given in (5.1b) below and  $\hat{K}(\text{conv})$  by (2.26b)] and the spin-independent kernels from two Coulomb exchanges—all of which contribute in  $O(\alpha^4)$ . Similarly, the matrix elements involving derivatives with respect to  $E'$  in the second and third terms of (2.13b) must be  $O(\alpha^2)$  in order to contribute. With the choice of  $\mathcal{V}$  in (2.15a), the matrix element of  $\partial\mathcal{V}/\partial E'$  is too small to contribute, as was explained at the end of Sec. II.A.  $\hat{K}(\text{spin})$  and  $\hat{K}(\text{conv})$  can contribute in the order of interest because the derivative can introduce an additional small denominator. As noted at the end of Sec. II.B, the term involving the derivative of  $\hat{K}(\text{conv})$  cancels a term arising from rearranging the sum over states.

In order to obtain a hyperfine splitting from the sum over states, we must have at least one matrix element involving  $\hat{K}(\text{spin})$ . Contributions involving one spin-independent matrix element and one spin-dependent matrix element were discussed in Sec. II.B, where they were shown to be canceled precisely by terms from Secs. III.B and IV.B.2. Thus we need analyze only the contributions containing two spin-dependent matrix elements.

We consider first the energy shift from the sum over states [fourth term of (2.13b)]

$$\Delta E(\text{state-sum}) = \sum_{n \neq 0} \frac{\langle \bar{0} | \hat{K}(\text{spin}) | \bar{n} \rangle \langle \bar{n} | \hat{K}(\text{spin}) | \bar{0} \rangle}{E_0 - E_n}, \quad (5.1a)$$

where the spin-dependent kernel we need is given by the last term of (2.23b)

$$\hat{K}(\text{spin}) = \frac{4\pi\alpha}{E'' + m_\mu} NV_c \bar{S} \frac{-i\alpha_e \cdot \sigma_\mu \times \mathbf{q}}{q^2} \bar{S} NV_c. \quad (5.1b)$$

Factors of  $\bar{S}NV_c$  adjacent to ground-state wave functions may be “absorbed into the wave function” using (2.24) (here one can neglect the difference between  $\mathcal{V}$  and  $NV_c$ ). Such factors adjacent to the state  $|\bar{n}\rangle$  are not rearranged using (2.24) because that would produce individual terms that contain spurious ultraviolet divergences. Instead, at this point we make a nonrelativistic reduction of the matrix element, which becomes

$$\langle \bar{n} | \hat{K}(\text{spin}) | \bar{0} \rangle = \frac{4\pi\alpha}{2E} \left\langle \bar{n} \left| V_c \frac{-1}{\mathbf{p}^2 + \gamma^2} \frac{\sigma_e \times \mathbf{q} \cdot \sigma_\mu \times \mathbf{q}}{q^2} \right| \bar{0} \right\rangle, \quad (5.2)$$

where the  $|\bar{n}\rangle$  are now Coulomb-Schrödinger states. Now, it turns out to be simplest to analyze this expression in coordinate space. For example,

$$\begin{aligned} 4\pi\alpha \frac{\sigma_e \times \mathbf{q} \cdot \sigma_\mu \times \mathbf{q}}{q^2} &\rightarrow \sigma_e \times \nabla \cdot \sigma_\mu \times \nabla V_c \\ &\doteq \frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle 4\pi\alpha \delta(\mathbf{r}) \\ &\quad + \frac{3\alpha}{r^3} (\sigma_e \cdot \hat{\mathbf{r}} \sigma_\mu \cdot \hat{\mathbf{r}} - \frac{1}{3} \sigma_e \cdot \sigma_\mu), \end{aligned} \quad (5.3)$$

where  $\hat{\mathbf{r}} = \mathbf{r}/|\mathbf{r}|$ . The first term in (5.3) connects the ground state to intermediate  $S$  states, the second to intermediate  $D$  states.

Let us first work out the  $s$ -state sum. For this we need

$$\frac{-1}{\mathbf{p}^2 + \gamma^2} \delta(\mathbf{r}) |\bar{0}\rangle = -\frac{1}{4\pi r} |\bar{0}\rangle. \quad (5.4)$$

This may be seen most easily by operating on (5.4) with  $\mathbf{p}^2 + \gamma^2$  and noting that the rhs is the solution which vanishes at spatial infinity. Inserting this into the sum over states, we find

$$\begin{aligned} \Delta E(S \text{ sum}) &= \langle (\sigma_e \cdot \sigma_\mu)^2 \rangle \frac{\alpha^4 m_r^2}{9m_e^2 m_\mu^2} \\ &\quad \times \sum_{n \neq 0} \frac{\langle \bar{0} | \frac{1}{r^2} | \bar{n} \rangle \langle \bar{n} | \frac{1}{r^2} | \bar{0} \rangle}{\epsilon_0 - \epsilon_n}. \end{aligned} \quad (5.5)$$

For the remainder of this section  $\epsilon_n$  represents the nonrelativistic approximation to the energy, including reduced-mass effects. Let us define  $f_s$  by

$$f_s = \sum_{n \neq 0} \frac{|\bar{n}\rangle \langle \bar{n} | \frac{1}{r^2} | \bar{0} \rangle}{\epsilon_0 - \epsilon_n}. \quad (5.6a)$$

Following Dalgarno and Lewis (1955), we note that  $f_s$  satisfies a differential equation:

$$\begin{aligned} \left[ \frac{-\gamma^2 + \nabla^2}{2m_r} - V_c \right] f_s(r) &= \frac{1}{r^2} |\bar{0}\rangle - |\bar{0}\rangle \left\langle \bar{0} \left| \frac{1}{r^2} \right| \bar{0} \right\rangle \\ &= \left[ \frac{1}{r^2} - 2\gamma^2 \right] \tilde{\phi}_{\text{nr}}(0) e^{-\gamma r}. \end{aligned}$$

The solution vanishing at infinity is

$$f_s = 2m_r (\ln \gamma r + \gamma r + b) \tilde{\phi}_{\text{nr}}(0) e^{-\gamma r}, \quad (5.6b)$$

where the constant  $b$  is fixed by the orthogonality condition

$$\begin{aligned} 0 &= \int_0^\infty f_s(r) \tilde{\phi}_{\text{nr}}(r) r^2 dr \\ &= 2m_r [\tilde{\phi}_{\text{nr}}(0)]^2 \int_0^\infty e^{-2\gamma r} (r^2 \ln \gamma r + \gamma r^3 + br^2) dr. \end{aligned} \quad (5.6c)$$

Substituting (5.6) into (5.5), we find that

$$\Delta E(S \text{ sum}) = \langle (\sigma_e \cdot \sigma_\mu)^2 \rangle \frac{2\alpha^4 |\tilde{\phi}_{nr}(0)|^2 m_r^3}{9m_e^2 m_\mu^2} \times \int_0^\infty 4\pi e^{-2\gamma r} (\ln \gamma r + b + \gamma r) dr. \quad (5.7a)$$

Integrating (5.6c) by parts twice and substituting in (5.7a) to eliminate  $b$ , we obtain

$$\Delta(S \text{ sum}) = \frac{10}{3} E_F \frac{\gamma^2}{m_e m_\mu}. \quad (5.7b)$$

Next we work out the  $D$ -state sum in a similar manner. The first step is

$$\begin{aligned} & \frac{-1}{\mathbf{p}^2 + \gamma^2} (\sigma_e \cdot \hat{\mathbf{r}} \sigma_\mu \cdot \hat{\mathbf{r}} - \frac{1}{3} \sigma_e \cdot \sigma_\mu) \frac{-3\alpha\gamma}{r^3} |\bar{0}\rangle \\ &= (\sigma_e \cdot \hat{\mathbf{r}} \sigma_\mu \cdot \hat{\mathbf{r}} - \frac{1}{3} \sigma_e \cdot \sigma_\mu) \frac{-3\alpha\gamma}{2r} |\bar{0}\rangle, \end{aligned} \quad (5.8)$$

which can be verified by writing the expression as a differential equation.

The next step is to work out the function  $f_d$ , defined by

$$(\sigma_e \cdot \hat{\mathbf{r}} \sigma_\mu \cdot \hat{\mathbf{r}} - \frac{1}{3} \sigma_e \cdot \sigma_\mu) f_d = \sum_{n \neq 0} \frac{|\bar{n}\rangle \langle \bar{n}| (\sigma_e \cdot \hat{\mathbf{r}} \sigma_\mu \cdot \hat{\mathbf{r}} - \frac{1}{3} \sigma_e \cdot \sigma_\mu) \frac{1}{r^2} |\bar{0}\rangle}{\epsilon_0 - \epsilon_n}, \quad (5.9a)$$

$$\begin{aligned} \langle \bar{0} | \frac{\partial N\hat{K}}{\partial E'} | \bar{0} \rangle &= -\frac{4\pi\alpha}{2E} \langle \bar{0} | \bar{S} \frac{-i\alpha_e \cdot \sigma_\mu \times \mathbf{q}}{q^2} + \frac{-i\alpha_e \cdot \sigma_\mu \times \mathbf{q}}{q^2} \bar{S} | \bar{0} \rangle \\ &= \frac{-4\pi\alpha \frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle}{2E} \langle \bar{0} | \delta(\mathbf{r}) \frac{-1}{\mathbf{p}^2 + \gamma^2} + \frac{-1}{\mathbf{p}^2 + \gamma^2} \delta(\mathbf{r}) | \bar{0} \rangle. \end{aligned} \quad (5.11a)$$

Using (5.4), we find that

$$\Delta E(\text{deriv}) = -\frac{4}{3} E_F \frac{\gamma^2}{m_\mu m_e}. \quad (5.11b)$$

The total energy shift from second-order perturbation theory due to two hyperfine interactions is then

$$\Delta E(\text{sum} + \text{deriv}) = (2 - \frac{1}{72}) E_F \frac{\gamma^2}{m_\mu m_e}. \quad (5.12)$$

As noted in the Introduction, this agrees with similar results obtained by Caswell and Lepage (1978a), even though there is not an exact correspondence between the terms calculated.

where  $f_d$  satisfies the differential equation

$$\begin{aligned} & -\frac{1}{2m_r} \left[ -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{6}{r^2} - \frac{2\gamma}{r} + \gamma^2 \right] f_d \\ &= \frac{1}{r^2} e^{-\gamma r} \tilde{\phi}_{nr}(0). \end{aligned} \quad (5.9b)$$

The solution vanishing at infinity is

$$f_d = -\frac{m_r}{3} \tilde{\phi}_{nr}(0) e^{-\gamma r}. \quad (5.9c)$$

Substituting these results into the sum over states, we find for the hfs contribution

$$\Delta E(D \text{ sum}) = -\frac{1}{72} E_F \frac{\gamma^2}{m_\mu m_e}. \quad (5.10)$$

Finally, we must calculate the second-order energy shift due to the  $\partial \hat{K} / \partial E'$  term [third term of (2.13b)]. All the  $E'$  dependence in (5.1b) is contained in  $\bar{S}$ , so the factor involving the derivative is

## VI. SUMMARY AND OUTLOOK

We review briefly our results, including radiative correction contributions where appropriate, and also discuss their implications for some related experiments. The outlook for further work is also described.

### A. Muonium hfs

The contributions not involving recoil were discussed at the end of Sec. III.D. To separate binding effects from radiative corrections, we use factors of  $Z\alpha$  for the former in the following expression:

$$\begin{aligned} \Delta E(\text{non-rec., incl. rad. corr.}) &= E_F (1 + a_\mu) \left[ 1 + \frac{3}{2} (Z\alpha)^2 + a_e + \alpha(Z\alpha) (\ln 2 - \frac{5}{2}) - \frac{8\alpha(Z\alpha)^2}{3\pi} \ln Z\alpha (\ln Z\alpha - \ln 4 + \frac{281}{480}) \right. \\ &\quad \left. + \frac{\alpha(Z\alpha)^2}{\pi} (15.38 \pm 0.29) + \frac{\alpha^2(Z\alpha)}{\pi} D_1 \right]. \end{aligned} \quad (6.1)$$



Note that we use  $E_F$  as defined in (1.1), so that an explicit factor of  $(1+a_\mu)$  appears here. See footnote 1. The  $\alpha(Z\alpha)$  radiative correction was calculated originally by Kroll and Pollock (1951,1952) and Karplus, Klein, and Schwinger (1951). A simpler method is given by Sapirstein, Terray, and Yennie (1984). The  $\alpha(Z\alpha)^2$  radiative corrections containing  $\ln\alpha$  were first calculated by Layzer (1961,1964) and Zwanziger (1961,1964). Brodsky and Erickson (1966) confirmed those terms and estimated the nonlogarithmic term. Very recently, the nonlogarithmic term was evaluated numerically by Sapirstein (1983). The  $D_1$  term represents uncalculated radiative corrections involving two virtual photons.

The recoil corrections discussed in this paper sum to

$$\Delta E(\text{rec}) = E_F \left[ -\frac{3\alpha}{\pi} \frac{m_e m_\mu}{m_\mu^2 - m_e^2} \ln \frac{m_\mu}{m_e} + \frac{\gamma^2}{m_e m_\mu} \left[ 2 \ln \frac{m_r}{2\gamma} - 6 \ln 2 + 3 \frac{11}{18} \right] \right]. \quad (6.2)$$

The first term in mass-symmetric form is due to Arnowitt (1953). The  $(\gamma^2/m_e m_\mu) \ln(m_r/2\gamma \approx 1/2\alpha)$  term was calculated by Lepage (1977) and by Bodwin and Yennie (1978). The other terms are new in the present work [first reported in Bodwin, Yennie, and Gregorio (1982)]. The muon's anomalous moment does not appear here, since its effect should be counted as part of the radiative-recoil correction.

The radiative-recoil contributions, which arise from both lepton lines and from vacuum polarization, are given by

$$\Delta E(\text{rad-rec}) = E_F \left[ \frac{\alpha}{\pi} \right]^2 \frac{m_e}{m_\mu} \left[ -2 \ln^2 \frac{m_\mu}{m_e} + \frac{13}{12} \ln \frac{m_\mu}{m_e} + (18.18 \pm 0.63) \right]. \quad (6.3)$$

The present importance of these terms was first pointed out by Caswell and Lepage (1978b), who evaluated the one proportional to  $\ln^2(m_\mu/m_e)$ . Terray and Yennie (1982) then evaluated the single  $\ln$  terms; an apparent change in the coefficient is due to our changed choice of conventions in writing these expressions. Finally, the additive contribution was calculated by Sapirstein, Terray, and Yennie (1983,1984). The hadronic vacuum polarization contribution is included; it contributes less than 2 to the final coefficient. Weak neutral-current effects are estimated to be less than 0.1 ppm [Bég and Feinberg (1974) and Bodwin and Yennie (1978)]. At the present time, these effects are negligible, which makes muonium a pure QED system to the present level of approximation.

We do not wish to give a detailed review of the place of muonium hfs in high-precision tests of QED, but a few comparisons may be enlightening. For a more complete survey, see a conference paper by Kinoshita and Sapirstein (1984). The theoretical expression, with the best values of the physical constants other than  $\alpha$ , may be

combined with the present experimental results of Mariam *et al.* (1982)

$$\nu = 4\,463\,302.88(16) \text{ kHz}$$

to yield a value of  $\alpha$ :

$$\alpha_{\text{hfs}}^{-1} = 137.035\,991(20)(15),$$

where the contributing uncertainties are 20 for the muon's mass (equivalently its magnetic moment) and 15 for  $D_1$ , which is assumed to contribute a 1-kHz uncertainty. The value of  $\alpha$  obtained by comparing the theory [Kinoshita and Lindquist (1981)] and experiment [Schwinberg, Van Dyck, and Dehmelt (1981)] for the electron's anomalous moment is

$$\alpha_{g-2}^{-1} = 137.035\,993(10).$$

Finally, the solid-state determination from the Josephson junction (Williams and Olsen, 1979,1984) is

$$\alpha_J^{-1} = 137.035\,963(15).$$

We do not present the quantized-Hall-effect result, which may be less sound.

### B. Positronium hfs

The theoretical expression for the positronium hfs is given by

$$\nu = \alpha^2 R_\infty \left[ \frac{2}{3} + \frac{1}{2} - \frac{\alpha}{\pi} (\ln 2 + \frac{16}{9}) + \frac{5}{12} \alpha^2 \ln \alpha^{-1} + K\alpha^2 + K'(\alpha)\alpha^3 \right].$$

The  $\alpha/\pi$  term includes radiative corrections as well as a term obtained by taking the equal-mass limit of (6.2). The  $\alpha^2 \ln \alpha^{-1}$  term comes partially from (6.2), but it has previously noted contributions from annihilation kernels (Barbieri and Remiddi, 1976; and Caswell and Lepage, 1979). The  $\alpha^2$  term has been only partially evaluated. Various contributions to  $K$  are: two-photon annihilation kernels: 1.408 (Cung *et al.*, 1978b); three-photon annihilation kernels:  $-0.098$  (Cung *et al.*, 1977,1978a); and the radiative-recoil corrections  $-1.079$  (Sapirstein, Terray, and Yennie, 1984). Recoil corrections of the type contained in (6.2) and also some two-photon radiative corrections in the one-photon annihilation channel remain to be done. The  $K'$  term is uncalculated, but it could be enhanced by factors of  $\ln \alpha$ .

The most recent experimental result by Ritter *et al.* (1984) is

$$\nu = 203\,389.10(74) \text{ MHz}.$$

The present theoretical value (Sapirstein and Kinoshita, 1984), including all known contributions, is

$$\nu = 203\,402.51 \text{ MHz}.$$

The difference between theory and experiment is quite

compatible with the expected magnitude of the uncalculated terms.

### C. Hydrogen hfs

The hfs for the hydrogen ground state is one of the most accurately measured quantities in physics (Hellwig *et al.*, 1970; Essen *et al.*, 1971):

$$\nu = 1420.405\,751\,766\,7(9) \text{ MHz}.$$

On the theoretical side, the result (6.1) can be applied directly to hydrogen by replacing the muon's anomalous moment by the proton's. Zemach's (1956) finite-proton-size correction, which is also proportional to the total magnetic moment of the nucleus, can also be added to the large parentheses of (6.1). The additional term is  $-2m_r\alpha R_{pr}$ , where  $R_{pr}$  is a mean radius associated with the proton's static charge-current distribution. The size of this effect is  $-38.2$  ppm. On the other hand, neither the first term of (6.2) nor all of (6.3) can be applied directly to the hydrogen hfs. The reason is that they are characterized by momenta between  $m_e$  and  $m_p$ , while the finite size of the proton cuts off the integrations at  $\approx m_\pi$ . These terms which combine recoil and finite size were first estimated by Arnowitt (1953) and by Newcomb and Salpeter (1955). With the measured elastic proton form factors, the complete finite-size contribution is changed to  $-34.6(9)$  ppm (Grotch and Yennie, 1967). The physical contributions which limit our ability to interpret the experimental value are the proton polarizability contributions, called  $\delta_p$ . Important progress has been made since the classic work of Iddings (1965). It will not be reviewed here, but we mention that deRafael (1971) and Gnädig and Kuti (1972) showed how to use data from inelastic electron scattering with polarized beam and target to put bounds on  $\delta_p$ . In a recent review, Hughes and Kuti (1983) give the upper bound  $|\delta_p| < 4$  ppm. If  $\delta_p$  is the only important correction, it would have to be  $+1.6(9)$  ppm to bring agreement between theory and experiment (of course its value and error could change if the determination of the complete finite size contribution is improved). If there is significant improvement in these results, the last term of (6.2) should be redone to include the proton's anomalous magnetic moment. As has been emphasized in the detailed analysis, this term comes from the low-momentum region [ $\gamma (\equiv am_r)$  to  $m_e$ ], so that the uncertainties from proton structure should be unimportant for it. This contribution is currently being evaluated by two of the present authors (Bodwin and Yennie, 1985).

### D. Outlook

What is the next stage in the analysis of contributions to muonium hfs? For the recoil corrections, our results seem to be adequate for a long time to come. The next steps required for more stringent tests are the calculation of  $D_1$  in (6.1) and the improvement of the measurement of the muon's mass. On the other hand, it is valuable to

check a calculation as complicated as the one presented here. This has recently been done by Caswell and Lepage (1985) who arranged the calculation quite differently and carried out the integrations numerically. Their result agrees with ours within their error of about 0.2 in the coefficient of  $\gamma^2/m_e m_\mu$ . They have also obtained the corresponding contributions for positronium. Similar work is in progress by Sapirstein (1984).

Should it become important to extend our calculation to higher order (in  $\alpha$ , since the numerical work is not restricted in powers of the mass ratio), we believe that our method could be generalized. In addition to picking up various small terms which we were able to neglect, it would of course be necessary to consider higher-order kernels. At that stage, we would find a new phenomenon (for this problem). The kernels themselves would become nonperturbative. That is, it would be necessary to consider kernels with an arbitrary number of Coulomb photons. This phenomenon is familiar from other problems such as the Lamb shift. Previous experience has been that such terms are tractable.

### ACKNOWLEDGMENTS

We benefited greatly in this work from many conversations with G. Peter Lepage, whose work has paralleled ours in many ways. We also wish to acknowledge helpful conversations with Tom Kinoshita and Jonathan Sapirstein. This work was initiated several years ago; and although it has undergone several changes of form, we should like to express our appreciation to those who gave us support during the whole period. One of us (D.R.Y.) was the recipient of a Guggenheim Fellowship during 1978–1979, for which he is most appreciative. During that year he enjoyed the hospitality of Université de Paris VI, Centre d'Etudes Nucléaires de Saclay, and CERN. Another of us (G.T.B.) received support through the University of Illinois and SLAC during earlier stages of this work. At Cornell, this work was supported in part by the National Science Foundation and at Argonne by the U.S. Department of Energy. One of us (M.A.G.) is a research fellow of the Conselho Nacional de Pesquisas (CNPq), Brasil. He is grateful to the NSF-CNPq Program for International Cooperation, since it allowed his participation in the present work.

### APPENDIX A: SIMPLE GUIDE FOR ORDER-OF-MAGNITUDE ESTIMATES

An important part of the technique of making bound-state calculations is the ability to identify terms of the order of interest and to make approximations which simplify the calculation. Generally, this is a skill which comes with experience, and it is difficult to give a set of rules which works in every situation. There are many paths to a correct result, and the difficulty of calculation is not path independent. A grasp of the general principles for determining orders of magnitude is invaluable for avoid-

ing various pitfalls. We attempt to provide an introduction to this subject here.

There is no straightforward procedure for making an expansion in powers of the small parameters  $\alpha$  and  $m_e/m_\mu$ ; the presence of terms in  $\ln\alpha$  and  $\ln(m_\mu/m_e)$  shows this. One cannot simply count vertices in a given kernel to determine the order in  $\alpha$ , because  $\alpha$  also occurs in the kernel propagators and in the wave function in the combination  $\gamma = m_e\alpha$ . Furthermore, one cannot arbitrarily expand the integrand in inverse powers of  $m_\mu$ : at some point the resulting integrals become divergent at large momenta.

A simple approach for estimating orders of magnitude is to use dimensional analysis for the different ranges of (spatial) momenta. One first carries out the loop energy integrals by contour integration. This may not be the best approach for the actual calculation, but it does help us in locating terms of different orders. Usually the contour is closed in such a way that positive-energy electron poles are not enclosed. This leaves negative-energy electron poles, photon poles, or muon poles. The important ranges of momenta to consider are

- (a) very low momenta:  $p \leq \gamma$ ,
- (b) low momenta:  $\gamma \leq p \leq m_e$ ,
- (c) intermediate momenta:  $m_e \leq p \leq m_\mu$ ,
- (d) high momenta:  $m_\mu \leq p$ .

In each of these ranges, one simplifies the integrand as appropriate and extracts an overall factor consisting of powers of  $\alpha$ ,  $\gamma$ ,  $m_e$ , and  $m_\mu$ . For example, in ranges (a) and (b), one approximates  $(m_e^2 + \mathbf{p}^2)^{1/2}$  by  $m_e$  and  $[(m_e^2 + \mathbf{p}^2)^{1/2} - m_e]$  by  $\mathbf{p}^2/2m_e$  to determine the dominant behavior. In ranges (b), (c), and (d), one neglects  $\gamma$  compared to  $\mathbf{p}$ ,  $m_e$ , and  $m_\mu$ . In ranges (c) and (d), one can use  $(m_e^2 + \mathbf{p}^2)^{1/2} \approx |\mathbf{p}|$ . The resulting factor has some power of each of the parameters  $\alpha$ ,  $\gamma$ ,  $m_e$ , and  $m_\mu$  and some dimension (in powers of mass).

We start by discussing the behavior of the integral as a whole. Our discussion will have to be refined later to take into account behavior of subintegrals. Since the complete expression (overall factor times integral) must have the dimensions of mass, we can deduce the dimension  $d$  of the integral for each range. For  $d < 0$ , the main contribution to the integral comes from the vicinity of the lower limit and we expect it to yield the following:

$$(b) \gamma^d; (c) m_e^d; (d) m_\mu^d.$$

Note that in region (b) the integral may produce inverse powers of  $\gamma$ . Region (a), which has been omitted from this enumeration, requires a few words of explanation. It can become important in connection with a photon pole when the photon spans several Coulomb interactions (this happens in the Lamb shift, for example). Then the momentum of that photon is characterized by the binding energy ( $\approx \alpha^2 m_e$ ) and the same final order is associated with any number of Coulomb interactions. Fortunately, this complication does not arise in the present work. It will in the future if it becomes necessary to proceed to higher orders in  $\alpha$ .

For  $d > 0$ , we expect the main contribution to the integral to come from the vicinity of the upper limit of the range. For range (d), this is infinity. This simply signals an inappropriate expansion in this range, since the original integrals are convergent. For  $d > 0$ , we have the following results:

$$(a) \gamma^d; (b) m_e^d; (c) m_\mu^d.$$

Usually one would arrange practical calculations so as not to have  $d > 0$  for the range (c) unless the resulting contribution is negligible in the order of interest. If an expansion produces non-negligible terms of this type, one would need to keep a more exact expression at an earlier stage.

For  $d = 0$ , the integral has the potential to produce logarithms:

$$(b) \left[ \ln \frac{m_e}{\gamma} \right]^{n_b}; (c) \left[ \ln \frac{m_\mu}{m_e} \right]^{n_c}.$$

The dimension  $d = 0$  for range (d) indicates an improper expansion which should be avoided at an earlier stage in the analysis.

The preceding estimates give the orders of the leading contributions from a given integral. Often expected contributions of a particular order are not realized in the final result because of cancellations between terms. Part of the art of doing these calculations is to anticipate such cancellations during the analysis of the integrand, rather than after the integration. This usually makes the analytic integration simpler. An example is the cancellation of the  $d = 0$  terms in the intermediate range in relative-order  $\alpha^2$  situations. This is known as the Caswell-Lepage cancellation (1978b) and is described in Sec. IV.

We remind the reader that these estimates are not procedures for calculating integrals. However, they are helpful for suggesting approximations. For example, suppose that the numerator has a factor  $(\mathbf{p}^2 + m_e^2)^{1/2}$  and that when this is approximated by  $m_e$ ,  $d = -2$  in ranges (b) and (c). Note that the approximation is actually not valid in range (c). Range (b) dominates the result and the integral produces a factor  $\gamma^{-2}$ . The correction to the approximation is  $\mathbf{p}^2/[m_e + (\mathbf{p}^2 + m_e^2)^{1/2}]$ . In range (b), this may be approximated by  $\mathbf{p}^2/2m_e$ , which now gives  $d = 0$  and suggests a contribution  $\ln(m_e/\gamma)$  [smaller by a factor  $(\gamma/m_e)^2 \ln(m_e/\gamma)$  than the original result]. In range (c), one could approximate the correction by  $|\mathbf{p}|$ , which gives  $d = -1$  and produces a result smaller than the main contribution from range (b) by relative order  $\gamma^2/m_e^2$ . In summary, one could first approximate by  $m_e$ . This presumably gives a simpler integral than with  $(\mathbf{p}^2 + m_e^2)^{1/2}$ . Even though the approximation is inaccurate in the range (c), the error is of higher order than the term obtained. The correction is given by  $\mathbf{p}^2/[m_e + (\mathbf{p}^2 + m_e^2)^{1/2}]$  over the whole range. However, if one wishes only to calculate the more important logarithmic term  $(\gamma/m_e)^2 \ln(m_e/\gamma)$ , the correction term may be replaced with  $\mathbf{p}^2/2m_e$  and the integration restricted to the range (b).

Very frequently, subintegrations converge in a different

momentum range than is suggested by the overall properties of the integral. For example, suppose that  $d = -1$ , but that the wave functions are decoupled; we will describe how that can happen later. Then the integrals over wave-function momenta may be done separately. For  $S$ -state Coulomb wave functions, this produces a factor  $\gamma^{-1}$ . Thus from range (b) we obtain a factor  $\gamma^{-2}$  in place of the expected  $\gamma^{-1}$ . Further, the remaining integrals internal to the kernel now have  $d = +1$ , so they produce a factor of  $m_e$  from this range. The contribution is larger by a factor of  $m_e/\gamma \approx 1/\alpha$  than had been expected from the overall estimate.

It is obviously very important to notice when the wave-function integrals can be decoupled to yield a larger contribution than expected from the overall estimate. This cannot happen, for example, when there are numerator powers of the wave-function momentum in the integrand [although it may still be convenient to make use of the decoupling equation (3.18a), (3.18b)]. If such numerator powers are absent, we can decouple the wave functions by neglecting their momenta inside the kernel [or in the case of Coulomb interactions, simply by doing the integration using (3.17)]. If such neglect of wave-function momenta in the kernel results in a reduction of the order expected from the overall estimate, then the correction obtained by taking the wave function momenta into account is generally of higher order, since the wave function cannot be decoupled in the correction term.

## APPENDIX B: ALGEBRAIC REARRANGEMENT OF FEYNMAN INTEGRANDS

The first step in the calculation of higher-loop contributions is to combine the integrands of related contributions. We find in practice that this eliminates many spurious contributions of various sorts and leads to simplifications in the final integrations. The integrands to be combined correspond to the set of diagrams in which the photons are inserted into the muon lines in all ways.

A few words about our general strategy may be helpful. While we are prepared to take into account the large mass ratio where it is essential for simplicity, we try not to make this approximation at too early a stage. The first terms we drop are those which would not contribute to either positronium or muonium because they have too many powers of  $\alpha$ . The next are ones which have an additional factor of  $m_e/m_\mu$  beyond the order of interest, provided they do not accompany  $\ln\alpha$ . We are not strict about this; if it is easy to preserve the mass symmetry, we do it.

There are two useful rearrangements of the muon denominator which we shall use frequently:

$$\frac{1}{D_\mu(Q)} = \frac{1}{2E(Q_0+i\epsilon)} \left[ 1 - \frac{D_e(-Q)}{D_\mu(Q)} \right] \quad (\text{B1a})$$

$$= \frac{1}{2(E''-E')(Q_0+i\epsilon)} \left[ 1 - \frac{D_e(Q)}{D_\mu(Q)} \right]. \quad (\text{B1b})$$

The first form is particularly useful when  $Q$  is the negative of the four momentum in one of the electron lines; this would occur in a ladder structure. Then the first term can be rearranged as in (2.2d) to give a piece which fixes  $p_0$  plus a piece which gives a much smaller contribution, and the second term in (B1a) has a numerator which cancels out the electron denominator. The result of this rearrangement is

$$\frac{1}{D_\mu(-p)} = \frac{1}{2E} \left[ -2\pi i \delta(p_0) - \frac{1}{p_0+i\epsilon} - \frac{D_e(p)}{(-p_0+i\epsilon)D_\mu(-p)} \right]. \quad (\text{B1c})$$

The form (B1b) is sometimes more useful when there are crossed photon lines. Then the numerator of the second term usually has a piece which cancels an electron denominator. An example, with the particular labeling which will be used in VO, is

$$\frac{1}{D_\mu(p-p'-r)} = \frac{1}{2(E''-E')} \frac{1}{p_0-p'_0-r_0+i\epsilon} \times \left[ 1 - \frac{D_e(p)}{D_\mu(p-p'-r)} - \frac{(p-p'-r)^2-p^2}{D_\mu(p-p'-r)} \right]. \quad (\text{B1d})$$

An alternative option is to use (B1a) with crossed photon lines. Then we find

$$\frac{1}{D_\mu(p-p'-r)} = \frac{1}{2E} \frac{1}{p_0-p'_0-r_0+i\epsilon} \times \left[ 1 + \frac{D_e(p)}{D_\mu(p-p'-r)} - \frac{(p-p'-r)^2+p^2-2\gamma^2}{D_\mu(p-p'-r)} \right]. \quad (\text{B1e})$$

With crossed photon lines we have tried both forms of (B1d) and (B1e) to find the one that leads most directly to a useful result for the subsequent calculations. Here, of course, we present the form which is most convenient in each case. For the applications to follow, (B1d) and (B1e) simplify, because either one of  $p'_0$  and  $r_0$  vanishes or both of them do.

### 1. One-V contributions

The one-V contribution, complete to two intrinsic  $p_0$  integrations, is defined in Fig. 7. However, rather than deal with all these contributions at one time, we follow the procedure described in Sec. III.C to extract a sequence of terms of increasing complexity. Thus the leading-order contribution to the hfs arises from the one-V exchange which is defined and treated in Sec. III.D. VO and OV are defined by the one-loop graphs of Fig. 7, taken with a

positive sign. The [VO] + [OV] contribution is defined as a suitable portion of the complete VO + OV contribution with exactly twice the V contribution removed. Certain parts of the complete VO + OV expression have spurious divergences and are best not considered at this level. As they arise, we denote them by (VO) with various subscripts. The [OV] + [VO] contribution is dominated by the one-loop term treated in Sec. III.E. It has additional contributions which are essentially two-loop terms and are treated in Sec. IV.A.1. Next we proceed to sets like VOO and extract V and [VO] from them to leave [VOO] plus additional spurious terms and terms beyond the order of interest. At the end, many of the spurious terms cancel within the set of one-V contributions and others are left to compensate terms from the two-V graphs.

Our general procedure will be to study these kernels as Feynman integrals and at an appropriate point in the analysis identify the lower-order contributions which are to be removed. This does not prove to be difficult. The procedure is based on identities like (B1), but occasionally we shall invent other ones which lead to more tractable expressions for the final integrals.

In the following, we use a symbol  $\doteq$  to denote a simplification of an expression. It has two meanings. The most

important is that the hfs content is preserved. In addition, it may mean that we have dropped terms which have more powers of  $\alpha$  or of  $(m_e/m_\mu)$  than are presently under consideration. Usually we try to point out the latter approximations as we go along.

a. VO contribution

The electron factor is

$$\frac{\psi(\mathbf{p}')(E' + \beta_e m_e + p_0 + \alpha_e \cdot \mathbf{p})\psi(\mathbf{r})}{D_e(p)} \doteq \frac{\phi_{nr}^\dagger(\mathbf{p}')[\Omega_e + p_0 \Omega'_e / (m_e + E')] \phi_{nr}(\mathbf{r})}{D_e(p)}, \quad (B2a)$$

where we have used the fact that once the leading-order contribution has been removed, the Dirac wave function may be approximated using the nonrelativistic Coulomb wave function. Terms with four factors of  $\alpha_e$  are too small, since they would give one factor of  $\alpha$  beyond the present order of interest. Here

$$\Omega_e \equiv \alpha_e \cdot (\mathbf{p} - \mathbf{r}) \alpha_e, \quad \Omega'_e \equiv \alpha_e \cdot (\mathbf{p}' - \mathbf{r}) \alpha_e. \quad (B2b)$$

The muon factor for the ladder graph is given by

$$\frac{\left[1 - \frac{\alpha_\mu \cdot \mathbf{p}'}{m_\mu + E''}\right] (E'' + \beta_\mu m_\mu - p_0 - \alpha_\mu \cdot \mathbf{p}) \alpha_\mu \left[1 - \frac{\alpha_\mu \cdot \mathbf{r}}{m_\mu + E''}\right]}{D_\mu(-p)} \doteq \frac{\Omega_\mu - p_0 \Omega'_\mu / (m_\mu + E'')}{D_\mu(-p)}, \quad (B3a)$$

where we recall that in the reduction of the original kernels the decomposition (2.21) was used. In going from the exact to the approximate form, we have dropped terms which are negligible for muonium (factor of  $m_e/m_\mu$  beyond the present order of interest). They would contribute for positronium if taken with the  $\delta(p_0)$  part of the denominator rearrangement. They are the counterpart of electron terms which give part of the contribution to  $\frac{3}{2}\alpha^2$  in (3.15b). The abbreviations appearing in (B3a) are

$$\Omega_\mu \equiv -\alpha_\mu \cdot (\mathbf{p} - \mathbf{r}) \alpha_\mu, \quad \Omega'_\mu \equiv -\alpha_\mu \cdot (\mathbf{p}' - \mathbf{r}) \alpha_\mu. \quad (B3b)$$

The crossed graph muon factor is

$$\frac{\left[1 - \frac{\alpha_\mu \cdot \mathbf{p}'}{m_\mu + E''}\right] \alpha_\mu [E'' + \beta_\mu m_\mu + p_0 + \alpha_\mu \cdot (\mathbf{p} - \mathbf{p}' - \mathbf{r})] \left[1 - \frac{\alpha_\mu \cdot \mathbf{r}'}{m_\mu + E''}\right]}{D_\mu(p - p' - r)} \doteq \frac{\Omega_\mu + p_0 \Omega'_\mu / (m_\mu + E'')}{D_\mu(p - p' - r)}. \quad (B4)$$

Terms which have been dropped here are negligible for positronium as well as for muonium at the present level of interest. From now on in presenting other muon factors, we shall simply give the approximate form valid to the order of interest.

Next we consider the product of the electron and muon factors. It is convenient to arrange this according to the different structures appearing in the numerators.

(i)  $\Omega_e \cdot \Omega_\mu$ . The steps in the reorganization of these contributions will be described in considerable detail as an illustration of the methods used; subsequently other contributions will be outlined more compactly. We use (B1c) to rearrange the ladder muon denominator. Most of the  $\delta(p_0)$  term is to be deleted, since it is already incorporated in the V contribution. An additional piece arises from the  $V'_e$  term in (2.24); we call this piece (VO)<sub>1</sub>. From the discussion of Sec. II.B, we expect that this should be canceled by a piece of the VV contribution when we take the convection part of one of the photons. In fact, we can arrange this to happen, so this term need never be calculated. This compensating term is noted in Sec. IV.B.1. The remainder of the ladder muon denominator yields new contributions, which we must calculate. For the crossed graph contribution, we could use either of the forms (B1d) or (B1e) to obtain our ultimate objective. At this point, it seems more convenient to use the second of these again, since it leads to a number of immediate cancellations against terms in the ladder graph contribution (B1c).

The nonrecoil pieces from these expressions are seen to cancel each other directly. This type of cancellation is precisely the reason we choose to treat these sets of graphs together in this manner. At this stage, the sum of (B1c) and (B1e) times the electron factor may be written

$$\frac{\Omega_e \cdot \Omega_\mu}{2E} \left[ -\frac{1}{(-p_0 + i\epsilon)D_\mu(-p)} + \frac{1}{(p_0 + i\epsilon)D_\mu(p - p' - r)} - \frac{2(p - p')^2 + 2(\mathbf{p}' - \mathbf{r}) \cdot (\mathbf{p}' - \mathbf{p}) - r^2 - \mathbf{p}'^2 - 2\gamma^2}{(p_0 + i\epsilon)D_e(p)D_\mu(p - p' - r)} \right]. \tag{B5a}$$

This expression is not obviously symmetric in the masses, but we can make some variable transformations to bring out the symmetry. In the first term, we change the sign of  $p_0$ . In the second term we use  $\mathbf{p} \rightarrow \mathbf{p}' + \mathbf{r} - \mathbf{p}$  together with  $\mathbf{r} \leftrightarrow \mathbf{p}'$ ; the other factors in the complete expression are preserved under this transformation. The first two terms then cancel identically. Using the same vector transformation, we see that the last term is mass symmetric.

Now we replace the last term of (B5a) with a different one which is analytically simpler and also mass symmetric, and which gives the same hfs in muonium to the order of interest. We approximate the denominator by setting  $\mathbf{p}'$  and  $\mathbf{r}$  equal to zero. The corrections to this modification would have to be taken into account for positronium. Now we apply (B1b) to the last term and find

$$-\frac{\Omega_e \cdot \Omega_\mu}{4(m_\mu^2 - m_e^2)} \frac{2(p - p')^2 + 2\mathbf{p}' \cdot (\mathbf{p}' - \mathbf{p}) - 2\mathbf{r} \cdot \mathbf{p}' + 2\mathbf{p} \cdot \mathbf{r} - (r^2 + \gamma^2) - (\mathbf{p}'^2 + \gamma^2)}{(p_0 + i\epsilon)^2} \left[ \frac{1}{D_e(p)} - \frac{1}{D_\mu(p)} \right]. \tag{B5b}$$

The next thing to observe is that the  $(r^2 + \gamma^2)$  and  $(\mathbf{p}'^2 + \gamma^2)$  terms in the numerator of (B5b) are an artifact of the particular way we made the separation in (2.2c) for  $p'$  and  $r$ . Had we elected to put the muon on mass shell (in the lines containing  $p'_0$  and  $r_0$ ), the energy flow through the muon line in the crossed graph would have been altered by an amount which would have eliminated these terms from (B5b). While this might seem to be an argument in favor of putting the muon on mass shell (leading to the Gross equation), we recall that such a procedure has other undesirable consequences (see Sec. II.B). It is possible that there is some other option which will be more useful than either of these; anyone wishing to extend our calculation should keep that possibility in mind. The point we wish to make here is that these terms should not be treated as part of [VO]; in fact, to do so would lead to complications. Instead we now set them aside. These terms are properly a part of the two  $p_0$ -loop analysis. Thus we recall them when we deal with VOO and OVO, where they are largely canceled by other contributions which arise there. The expression for them is recorded here for later use:

$$\Omega_e \cdot \Omega_\mu \frac{(r^2 + \gamma^2) + (\mathbf{p}'^2 + \gamma^2)}{4(m_\mu^2 - m_e^2)(p_0 + i\epsilon)^2} \left[ \frac{1}{D_e(p)} - \frac{1}{D_\mu(p)} \right]. \tag{B5c}$$

The contribution which is part of [VO] is

$$-\Omega_e \cdot \Omega_\mu \frac{2(p - p')^2 + 2\mathbf{p}' \cdot (\mathbf{p}' - \mathbf{p}) - 2\mathbf{r} \cdot (\mathbf{p}' - \mathbf{r})}{4(m_\mu^2 - m_e^2)(p_0 + i\epsilon)^2} \times \left[ \frac{1}{D_e(p)} - \frac{1}{D_\mu(p)} \right]. \tag{B5d}$$

(ii)  $\Omega' \cdot \Omega$  ( $\doteq \Omega'_e \cdot \Omega_\mu$  or  $\Omega_e \cdot \Omega'_\mu$ ). Here we need only sketch the treatment, since it has many of the previous ingredients. The total contribution is obtained by taking the first numerator factor from the electron with the second from the muon and vice versa. Since the factor of  $p_0$  eliminates low-order contributions, we may make the

simplifications  $E' \approx m_e$  and  $E'' \approx m_\mu$ . We use (B1a) for the ladder graph contribution and (B1d) for the crossed graph, noting that  $p'_0 = r_0 = 0$ . In the resulting terms which have only one factor of  $D_e$  or  $D_\mu$ , the variable transformations which were introduced earlier are again used to simplify the result. Certain terms are extracted to be treated with [VO]:

$$\frac{\Omega' \cdot \Omega}{m_\mu^2 - m_e^2} \left[ \frac{1}{D_e(p)} - \frac{1}{D_\mu(p)} \right]. \tag{B6a}$$

In addition, there is a contribution

$$\Omega' \cdot \Omega \frac{(\mathbf{p} - \mathbf{p}' - \mathbf{r})^2 - \mathbf{p}^2}{4(E'' - E')m_r D_e(p)D_\mu(p - p' - r)}.$$

This may easily be seen to be symmetric in the masses with the help of the same variable changes used previously. We recast it into another form by first using (B1d). The second term of the new expression is transformed with the previously used variable change, and the last term is dropped. The dropped term is unimportant for muonium, but could contribute to positronium. The result is

$$\Omega' \cdot \Omega \frac{(\mathbf{p} - \mathbf{p}' - \mathbf{r})^2 - \mathbf{p}^2}{8(m_\mu^2 - m_e^2)m_r(p_0 + i\epsilon)} \left[ \frac{1}{D_e(p)} - \frac{1}{D_\mu(p)} \right]. \tag{B6b}$$

The role of this term is explained below.

(iii)  $\Omega'_e \cdot \Omega'_\mu$ . The reduction follows the same pattern, and we find a term to be included in [VO]:

$$\frac{\Omega'_e \cdot \Omega'_\mu p_0}{4E'E''(m_\mu^2 - m_e^2)} \left[ \frac{E''}{D_e(p)} - \frac{E'}{D_\mu(p)} \right]. \tag{B7}$$

We have dropped terms of higher order in  $m_e/m_\mu$  than is presently being considered.

To summarize the VO discussion, we have found the contributions (B5d), (B6a), and (B7) to be incorporated in

[VO]. The result, after angular averaging, is used in (3.16). We have set aside (B5c) and (B6b) to be treated with two-loop effects. We incorporate the part of them which is independent of  $\mathbf{r}$  into a term  $(VO)_2$  and the part independent of  $\mathbf{p}'$  into a term called  $(VO)_3$ . Other terms may be dropped. Our result for the analysis of VO is then

$$VO = V + [VO] + (VO)_1 + (VO)_2 + (VO)_3, \quad (B8)$$

where the final three "spurious" terms are explained in the text.

b. VOO contribution

The treatment we outline here applies in a similar way to OOV. We continue to follow the procedure explained in Sec. III.C. The electron and muon factors can again be expressed in terms of the  $\Omega$ 's [(B2b) and (B3b)]. New forms involving  $\mathbf{p}'' - \mathbf{r}$  also occur but their contributions are smaller than the present order of interest. The electron factor common to all graphs is

$$EF(VOO) \doteq \frac{\Omega_e(m_e + E' + p'_0) + \Omega'_e p_0}{D_e(p')D_e(p)}. \quad (B9)$$

The muon factors for the six graphs are

$$MF(VOO-1) \doteq \frac{\Omega_\mu(m_\mu + E'' - p'_0) - \Omega'_\mu p_0}{D_\mu(-p')D_\mu(-p)}, \quad (B10a)$$

$$MF(VOO-2) \doteq \frac{\Omega_\mu(m_\mu + E'' + p'_0 - 2p_0) + \Omega'_\mu p_0}{D_\mu(p' - p - p'')D_\mu(-p)}, \quad (B10b)$$

$$MF(VOO-3) \doteq \frac{\Omega_\mu(m_\mu + E'' + p'_0) - \Omega'_\mu p_0}{D_\mu(p' - p - p'')D_\mu(p' - p'' - r)}, \quad (B10c)$$

$$MF(VOO-4) \doteq \frac{\Omega_\mu(m_\mu + E'' - p'_0) + \Omega'_\mu p_0}{D_\mu(-p')D_\mu(p - p' - r)}, \quad (B10d)$$

$$MF(VOO-5) \doteq \frac{\Omega_\mu(m_\mu + E'' - p'_0 + 2p_0) - \Omega'_\mu p_0}{D_\mu(p - r - p'')D_\mu(p - p' - r)}, \quad (B10e)$$

$$MF(VOO-6) \doteq \frac{\Omega_\mu(m_\mu + E'' + p'_0) + \Omega'_\mu p_0}{D_\mu(p - r - p'')D_\mu(p' - p'' - r)}. \quad (B10f)$$

We have not discovered an approach to the analysis of the algebra of (B10) which is not rather tedious. In hopes of sparing the reader some of this tedium, we present a simplified derivation of an expression which is sufficiently accurate for our purposes. In fact, a rather elaborate analysis is necessary in order to justify the final result.

Here we present a very brief qualitative discussion of the nature of the subtleties which occur and the general methods which we have discovered to deal with them. Recall that our aim is to capture all contributions to order  $\alpha^2 E_F$  which contain  $\ln\alpha$  (regardless of the mass dependence) or which are leading order in the recoil for muonium. In order to obtain the  $\ln\alpha$  terms correctly, we may not make an expansion in powers of  $1/m_\mu$  at first; but after such terms are removed, we may proceed with such an expansion. We find in this way the leading terms which are to be calculated.

The difficulty is that the remainder terms in the expansion lead to very complicated integrals for which the simple discussion of Appendix A does not readily apply. Their structure is such that in some variables they have a low momentum sensitivity (producing a  $\ln\alpha$ ) and in other variables a high momentum sensitivity (producing terms of the same order in  $m_e/m_\mu$  as those kept). In the absence of further analysis, this state of affairs certainly would reduce our confidence in the results obtained by ignoring the remainders.

Another feature of our shortcut approach is that the terms we keep are not symmetric in the particle masses. This is not surprising, since the set of graphs VOO cannot provide such symmetry. However, it suggests that we ought to consider the complete set  $VOO + OVO + OOV$  as a unit. When we do this, the algebraic results are not manifestly mass symmetric, because the decomposition (B1) singles out the muon line. But, by a rather elaborate procedure involving variable transformations and regroupings of terms, we can restore the mass symmetry. More importantly, the sensitive integrals disappear, so that the results to be given here are justified. The reader can undoubtedly appreciate that such details are inappropriate in an expository paper of this type. After these remarks, we shall not refer to these difficulties, but simply carry out the analysis as we have announced. It is necessary to remember that at certain points we have used the small mass ratio  $m_e/m_\mu$  to avoid unpleasant terms. Thus many of the expressions are not applicable to positronium.

Some special features of order-of-magnitude estimates are described here briefly; an overview of such estimates is provided in Appendix A. The terms we must be most careful of in (B10) are those containing denominators  $D_\mu(-p')$  and/or  $D_\mu(-p)$ , since they contain the  $\delta(p'_0)$  and  $\delta(p_0)$  terms. Once we have isolated these terms, we can treat the remainder and all terms not containing  $D_\mu(-p)$  or  $D_\mu(-p')$  on an equal footing. When the  $p_0$  and  $p'_0$  contour integrations are carried out, the contributions arise from negative-energy electron or muon poles or photon poles. In such cases, the resulting integrand contains several (at least three) inverse powers of mass in the small-momentum region. The arguments of Appendix A then suggest that the wave-function momenta inside the loops can be neglected and that the wave-function integrals converge separately, as in (3.17a).

The first step is to identify the  $\delta(p'_0)$  terms, which occur in the first and fourth graphs. Of course, most of

these terms have already been encountered in the study of VO. The VO terms are easily identified by using (B1c) for  $D_\mu(-p')$ , where they are associated with the first term on the right-hand side. [Again we find a term involving  $V'_e$  from the use of (2.24); we call this term (VOO)<sub>1</sub>. As in the case of a similar term in VO, this one is exactly compensated by a convection contribution from a V photon; the compensation is noted in Sec. IV.B.3.] Rather than use the breakdown (B8) for this VO term, we elect to treat the (VO)<sub>2</sub> part as a part of [VOO]. This term is really an artifact of the particular method used to treat the muon pole [see the discussion following (B5b)]

and it cancels when all the  $\delta(p'_0)$  terms are taken into consideration. The (VO)<sub>1</sub> and (VO)<sub>3</sub> parts of (VO) are left over.

The second main step is to identify the terms containing a factor of  $\delta(p_0)$ . These arise from the first and second graphs. In the first graph, we have already extracted the  $\delta(p'_0)$  part, so we keep only the last two terms of (B1c). For the denominator  $D_\mu(-p)$ , we start with the first term of (B1c) and consider the part of the muon factor proportional to  $\Omega_\mu$ . This yields the contribution (for both graphs)

$$\frac{-2\pi i \delta(p_0) \Omega_\mu}{2E} \left[ \frac{-(2E'' - p'_0)}{2E} \left( \frac{1}{p'_0 + i\epsilon} + \frac{D_e(p')}{(-p'_0 + i\epsilon) D_\mu(-p')} \right) + \frac{(2E'' + p'_0)}{D_\mu(p' - p'' - p)} \right]. \quad (\text{B11a})$$

From now on, we may safely use the approximation  $E' \approx m_e$  and  $E'' \approx m_\mu$ . We rearrange the last denominator of (B11a) using (B1e), with a change of argument. Then in the terms which have a factor of  $D_e(p')$  in the numerator, we use symmetry to simplify the resulting expression, and rewrite the product of electron and muon factors as

$$\frac{-2\pi i \delta(p_0) \Omega_e \cdot \Omega_\mu}{4E^2 D_e(p)} \left[ \frac{2(2m_e + p'_0)}{D_e(p')} + \frac{2(2m_\mu + p'_0)}{D_\mu(p')} - \frac{(2m_e + p'_0)(2m_\mu + p'_0)[2(p' - p'') \cdot (p' - p) - \mathbf{p}^2 - \mathbf{p}''^2 - 2\gamma^2]}{(p'_0 + i\epsilon) D_e(p') D_\mu(p' - p'' - p)} \right]. \quad (\text{B11b})$$

In the last numerator of this expression, we drop the contribution  $\mathbf{p}''^2 + \gamma^2$ , which should enter only at the next level of approximation. There we expect it to cancel. This is analogous to the behavior of the  $\mathbf{p}^2 + \gamma^2$  term, which as we shall see, cancels at the present level. Also, the  $\mathbf{p}''$  and  $\mathbf{p}$  dependence in the denominator will be dropped, since the correction would have additional inverse powers of  $m_\mu$ . At this point the denominator of this last term is rearranged using (B1b); and with some further juggling, we may rewrite the main terms as

$$\frac{-2\pi i \delta(p_0) \Omega_e \cdot \Omega_\mu}{4E(m_\mu^2 - m_e^2) D_e(p)} \left[ \frac{2m_\mu(2m_e + p'_0)}{D_e(p')} + \frac{4m_e m_\mu [2(\mathbf{p}' - \mathbf{p}'') \cdot (\mathbf{p}' - \mathbf{p}) + \mathbf{p}^2 + \gamma^2]}{2(p'_0 + i\epsilon)^2 D_e(p')} + \frac{(2E + p'_0)(\mathbf{p}'^2 - 2\mathbf{p} \cdot \mathbf{p}')}{2(p'_0 + i\epsilon) D_e(p')} - (m_e \leftrightarrow m_\mu) \right]. \quad (\text{B11c})$$

Except for the second term in the large parentheses, we can ignore  $\mathbf{p}''$  and  $\gamma$  dependence in the numerators to the present order of interest. We define a part of this to be incorporated into the [VOO] contribution, namely,

$$\frac{-2\pi i \delta(p_0) \Omega_e \cdot \Omega_\mu}{4E(m_\mu^2 - m_e^2) D_e(p)} \left[ \frac{2m_\mu(2m_e + p'_0)}{D_e(p')} + \frac{4m_e m_\mu (\mathbf{p}' - \mathbf{p}'') \cdot (\mathbf{p}' - \mathbf{p})}{(p'_0 + i\epsilon)^2 D_e(p')} - (m_e \leftrightarrow m_\mu) \right]. \quad (\text{B12})$$

At this stage, we have taken into account contributions from the first term of (B1c), as applied to (B10a), (B10b), and (B10d). Now we describe the treatment of the remaining contributions from (B10a), (B10b), and (B10d), as well as the contributions from other terms of (B10). We again use (B1) in this simplification and retain only terms of the order of interest. Obviously, this leads to quite lengthy expressions which we do not reproduce here. We draw attention only to one subtlety. The last term of (B1c) appears to behave dominantly like  $\delta(p_0$  or  $p'_0)$ . However, in association with factors from the other muon propagator, it turns out to give additional  $\delta(p_0$  or  $p'_0)$  contributions, part of which cancel the (VO)<sub>2</sub> term mentioned previously. One simplification is that we can now drop all terms which are of higher order in  $m_e/m_\mu$  without affecting the coefficient of  $\ln \alpha$ . As discussed after (B10), this is not self-evident; but it is true. The result of this analysis is

$$\frac{1}{4m_\mu^2 D_e(p) D_e(p')} \left[ \Omega_e \cdot \Omega_\mu 2\mathbf{p}' \cdot \mathbf{p} \left[ \frac{-2m_e 2\pi i \delta(p_0 - p'_0)}{(p_0 + i\epsilon)^2} + \frac{2\pi i [\delta(p_0) - \delta(p_0 - p'_0)]}{p'_0 + i\epsilon} \right] + \Omega_e \cdot \Omega' \left[ 2(2m_e + p'_0) 2\pi i \delta(p'_0 - p_0) + \frac{2\mathbf{p} \cdot \mathbf{p}' 2\pi i [\delta(p'_0) - \delta(p'_0 - p_0)]}{p_0 + i\epsilon} \right] + 2\Omega_e' \cdot \Omega_\mu p_0 2\pi i \delta(p_0 - p'_0) \right]. \quad (\text{B13})$$



After spin averaging, we transfer these results to Sec. IV.A.2, where (B12) yields the  $J_\beta$  terms, and (B13) gives the  $M$  contribution. Schematically, what we have accomplished is the following:

$$VOO = V + [VO] + [VOO] + (VOO)_1 + (VO)_1 + (VO)_3 . \tag{B14}$$

c. OVO contribution

The discussion of OVO follows the same pattern as that of OOV. Therefore we only outline the steps in the reduction of the raw integrands. It is necessary to introduce two new numerator structures,  $\Omega_e''$  and  $\Omega_\mu''$

$$\Omega_e'' = \alpha_e \cdot (\mathbf{p} - \mathbf{r}') \alpha_e , \tag{B15}$$

$$\Omega_\mu'' = -\alpha_\mu \cdot (\mathbf{p} - \mathbf{r}') \alpha_\mu .$$

These structures occur in OV, which we have not displayed explicitly. Now the electron factor is

$$EF(OVO) = \frac{(m_e + E')\Omega_e + p_0\Omega_e' + r_0\Omega_e''}{D_e(p)D_e(r)} . \tag{B16}$$

The muon factors for the six graphs are

$$MF(OVO-1) = \frac{(m_\mu + E'')\Omega_\mu - p_0\Omega_\mu' - r_0\Omega_\mu''}{D_\mu(-p)D_\mu(-r)} , \tag{B17a}$$

$$MF(OVO-2) = \frac{(m_\mu + E'' - r_0)\Omega_\mu + (p_0 - r_0)\Omega_\mu'}{D_\mu(p - p' - r)D_\mu(-r)} , \tag{B17b}$$

$$MF(OVO-3) = \frac{(m_\mu + E'' + p_0)\Omega_\mu + (p_0 - r_0)\Omega_\mu''}{D_\mu(p - p' - r)D_\mu(p - p' - r')} , \tag{B17c}$$

$$MF(OVO-4) = \frac{(m_\mu + E'' - p_0)\Omega_\mu + (r_0 - p_0)\Omega_\mu''}{D_\mu(-p)D_\mu(r - p - r')} , \tag{B17d}$$

$$MF(OVO-5) = \frac{(m_\mu + E'' + r_0)\Omega_\mu + (r_0 - p_0)\Omega_\mu'}{D_\mu(r - r' - p')D_\mu(r - p - r')} , \tag{B17e}$$

$$MF(OVO-6) = \frac{(m_\mu + E'')\Omega_\mu + p_0\Omega_\mu' + r_0\Omega_\mu''}{D_\mu(r - r' - p')D_\mu(p - r' - p')} . \tag{B17f}$$

Since the analysis of OVO parallels that of VOO, we need give only a brief indication of some of the intermediate steps. As before, the first step is to identify the  $\delta(r_0)$  terms in the first and second pieces of  $MF$  and the  $\delta(p_0)$  terms in the first and fourth pieces of  $MF$ . Most of these are identified as contributions discussed in connection with VO and OV. The  $(VO)_3$  and  $(OV)_3$  parts of these contributions are incorporated into [OVO]. At this point, we note that wave-function momenta ( $\mathbf{p}'$  and  $\mathbf{r}'$ ) may be neglected in all denominators of the remaining terms. The discussion of the  $\delta(r_0$  or  $p_0)$  contributions parallels that of the similar terms in VOO. The final result which leads to [OVO] is then

$$\frac{1}{4E^2D_e(p)D_e(r)} 2\mathbf{p} \cdot \mathbf{r} \left[ \frac{\Omega \cdot \Omega' 2\pi i [\delta(r_0) - \delta(r_0 - p_0)]}{p_0 + i\epsilon} + \frac{\Omega \cdot \Omega'' 2\pi i [\delta(p_0) - \delta(r_0 - p_0)]}{r_0 + i\epsilon} \right] . \tag{B18}$$

After spin averaging, this result is reported in Sec. IV.A.3.

The complete decomposition of OVO is thus

$$OVO = V + [VO] + [OV] + [OVO] + (VO)_1 + (OV)_1 + (VO)_2 + (OV)_2 . \tag{B19}$$

d. Summary of one-V terms

We can now see how some of the spurious terms cancel when we combine the expressions (B8), (B14), and (B19):

$$VOO + OVO + OOV - VO - OV = V + [VO] + [OV] + [VOO] + [OVO] + [OOV] + (VO)_1 + (OV)_1 + (VOO)_1 + (OOV)_1 . \tag{B20}$$

2. Two-V contributions

Two-V contributions are simpler than the one-V ones in that it is not necessary to identify and remove lower-order contributions. On the other hand, the reduction of the matrices needed in order to extract the hfs terms is somewhat more involved. As before, we start with the one-loop terms and extract as much as possible from them.

a. VV contribution

The analysis is arranged so as to identify the pure one-loop term first, but first it is necessary to rearrange the electron and muon factors. The electron factor is

$$\begin{aligned}
EF(VV) &= \frac{(E' + m_e + \boldsymbol{\alpha}_e \cdot \mathbf{p}') \alpha_{ei} (E' + \beta_e m_e + p_0 + \boldsymbol{\alpha}_e \cdot \mathbf{p}) \alpha_{ej} (E' + m_e + \boldsymbol{\alpha}_e \cdot \mathbf{r})}{(E' + m_e)^2 D_e(p)} \\
&\doteq \frac{p_0 \alpha_{ei} \alpha_{ej}}{D_e(p)} + \frac{C_{ij}^e}{(E' + m_e) D_e(p)}, \tag{B21a}
\end{aligned}$$

where

$$\begin{aligned}
C_{ij}^e &= \frac{(E' + m_e + \boldsymbol{\alpha}_e \cdot \mathbf{p}') \alpha_{ei} (E' + \beta_e m_e + \boldsymbol{\alpha}_e \cdot \mathbf{p}) \alpha_{ej} (E' + m_e + \boldsymbol{\alpha}_e \cdot \mathbf{r})}{E' + m_e} \\
&\doteq (\boldsymbol{\alpha}_e \cdot \mathbf{p}' \alpha_{ei} + \alpha_{ei} \boldsymbol{\alpha}_e \cdot \mathbf{p}) (\boldsymbol{\alpha}_e \cdot \mathbf{p} \alpha_{ej} + \alpha_{ej} \boldsymbol{\alpha}_e \cdot \mathbf{r}) - (\mathbf{p}^2 + \gamma^2) \alpha_{ei} \alpha_{ej} \\
&\equiv D_{ij}^e - (\mathbf{p}^2 + \gamma^2) \alpha_{ei} \alpha_{ej}.
\end{aligned}$$

The first term of the electron factor may also be written

$$\frac{p_0 \alpha_{ei} \alpha_{ej}}{D_e(p)} = \frac{\alpha_{ei} \alpha_{ej}}{2E'} - \frac{(p^2 - \gamma^2) \alpha_{ei} \alpha_{ej}}{2E' D_e(p)}. \tag{B21b}$$

It will be noted later that the first term of the rhs of (B21b) does not contribute to the hfs because of symmetries. Also, in the denominator, we may safely ignore the difference between  $m_e$  and  $E'$ . This permits us to replace the original electron factor with

$$EF(VV) \doteq \frac{-(p^2 - \gamma^2) \alpha_{ei} \alpha_{ej} + C_{ij}^e}{2m_e D_e(p)}. \tag{B21c}$$

The muon factor for the ladder graph is

$$\begin{aligned}
MF(VV; \text{ladder}) &= \frac{-p_0 \alpha_{\mu i} \alpha_{\mu j}}{D_\mu(-p)} + \frac{C_{ij}^\mu}{(m_\mu + E'') D_\mu(-p)} \\
&\doteq \frac{\alpha_{\mu i} \alpha_{\mu j}}{2m_\mu} + \frac{-(p^2 - \gamma^2) \alpha_{\mu i} \alpha_{\mu j} + C_{ij}^\mu}{2m_\mu D_\mu(-p)}. \tag{B22a}
\end{aligned}$$

In treating the muon factors, we ignore the difference between  $m_\mu$  and  $E''$  in the denominators. The expression for  $C_{ij}^\mu$  has some sign differences from  $C_{ij}^e$ , but the parts contributing to the hfs are the same. The muon factor for the crossed graph is

$$\begin{aligned}
MF(VV; \text{crossed}) &\doteq \frac{p_0 \alpha_{\mu j} \alpha_{\mu i}}{D_\mu(p - p' - r)} + \frac{E_{ji}^\mu}{2m_\mu D_\mu(p - p' - r)} \\
&\doteq \frac{\alpha_{\mu j} \alpha_{\mu i}}{2m_\mu} + \frac{-[(p - p' - r)^2 - \gamma^2] \alpha_{\mu j} \alpha_{\mu i} + E_{ji}^\mu}{2m_\mu D_\mu(p - p' - r)}, \tag{B22b}
\end{aligned}$$

where

$$\begin{aligned}
E_{ji}^\mu &= \frac{(E'' + m_\mu - \boldsymbol{\alpha}_\mu \cdot \mathbf{p}') \alpha_{\mu j} [E'' + \beta_\mu m_\mu + \boldsymbol{\alpha}_\mu \cdot (\mathbf{p} - \mathbf{p}' - \mathbf{r})] \alpha_{\mu i} (E'' + m_\mu - \boldsymbol{\alpha}_\mu \cdot \mathbf{r})}{E'' + m_\mu} \\
&\doteq [-\boldsymbol{\alpha}_\mu \cdot \mathbf{p}' \alpha_{\mu j} + \alpha_{\mu j} \boldsymbol{\alpha}_\mu \cdot (\mathbf{p} - \mathbf{p}' - \mathbf{r})] [\boldsymbol{\alpha}_\mu \cdot (\mathbf{p} - \mathbf{p}' - \mathbf{r}) \alpha_{\mu i} - \alpha_{\mu i} \boldsymbol{\alpha}_\mu \cdot \mathbf{r}] - [(\mathbf{p} - \mathbf{p}' - \mathbf{r})^2 + \gamma^2] \alpha_{\mu j} \alpha_{\mu i} \\
&\doteq -C_{ij}^\mu + 2(\mathbf{p}' + \mathbf{r})_j \alpha_{\mu i} \cdot (\mathbf{p}' - \mathbf{p}) \alpha_{\mu i} + 2(\mathbf{p}' + \mathbf{r})_i \alpha_{\mu j} \cdot (\mathbf{p} - \mathbf{r}) \alpha_{\mu j} - [(\mathbf{p} - \mathbf{p}' - \mathbf{r}) - \mathbf{p}^2] \alpha_{\mu j} \alpha_{\mu i}.
\end{aligned}$$

The final form of  $E_{ji}$  was obtained with the help of the following observation: for hfs terms, we may reverse the order of all  $\alpha$  matrices and change the overall sign. Note that the first terms of the second forms of the muon factors cancel each other for the hyperfine splitting. Similarly the first term of the rearranged form of the electron factor compensates by symmetry for the hfs (in the ladder graph use  $p_0 \rightarrow -p_0$  and in the crossed graph use  $\mathbf{p} - \mathbf{p}' - \mathbf{r} \rightarrow -\mathbf{p}$ ; the two contributions are the same except for interchange of  $i$  and  $j$ ). Dropping the canceling terms, we now rewrite the muon factors in the form which will be used in the subsequent analysis:

$$MF(VV; \text{ladder}) \doteq \frac{-(p^2 - \gamma^2)\alpha_{\mu i}\alpha_{\mu j} + C_{ij}^{\mu}}{2m_{\mu}D_{\mu}(-p)}, \tag{B22c}$$

$$MF(VV; \text{crossed}) = \frac{(p^2 - \gamma^2)\alpha_{\mu i}\alpha_{\mu j} - C_{ij}^{\mu}}{2m_{\mu}D_{\mu}(p - p' - r)} + \frac{2(\mathbf{p}' + \mathbf{r})_j \alpha_{\mu'}(\mathbf{p}' - \mathbf{p})\alpha_{\mu i} + 2(\mathbf{p}' + \mathbf{r})_i \alpha_{\mu'}(\mathbf{p} - \mathbf{r})\alpha_{\mu j}}{2m_{\mu}D_{\mu}(p - p' - r)}. \tag{B22d}$$

Before proceeding, we would like to approximate the denominator of (B22d) by neglecting  $\mathbf{p}'$  and  $\mathbf{r}$ . At first sight, this appears to be a perfectly acceptable approximation, since the correction contains an additional power of  $1/m_{\mu}$ . However, there is a small subtlety which we explain below.

We must be careful, since the correction to (B22d) may contain a sensitivity to low momenta which could lead to  $\ln\alpha$  terms. If we put the difference  $1/D_{\mu}(p - p' - r) - 1/D_{\mu}(p)$  over a common denominator, it appears that at low momentum the two muon denominators yield a factor  $(p_0 + i\epsilon)^2$ . If the  $p_0$  contour is closed in the upper-half-plane, the residue at the electron pole is innocuous, but the residues of the photon poles yield denominators cubic in one of the momentum transfers. Thus there may be a problem when  $\mathbf{p} \approx \mathbf{p}'$  or  $\mathbf{p} \approx \mathbf{r}$ . Terms with factors of  $p_0$  in the numerator are not a problem. We examine the second form of (B22b), with the second form of  $E_{ji}$ . Only the first term of  $E_{ji}$  (containing four factors of  $\alpha_{\mu}$ ) can cause a difficulty, since the second term cancels part of another piece of the numerator of (B22b), leaving only terms containing factors of  $p_0$ . The analysis of the electron factor is similar, and the conclusion is that only the first term in the second form of  $C_{ij}$  needs to be considered. Now in each factor of these remaining expressions we rearrange the alpha matrices into spin and convection pieces. The spin pieces have momentum differences  $\mathbf{p} - \mathbf{r}$  or  $\mathbf{p}' - \mathbf{p}$ . If we consider any contribution which has both of these factors, it cannot lead to any difficulty, since both photon factor singularities are cancelled. Therefore we study as an example the term which has two spin factors proportional to  $\mathbf{p}' - \mathbf{p}$ ; after spin averaging this leads to  $(\mathbf{p}' - \mathbf{p})^2$ . The other numerator factors combine to give a factor  $-2\mathbf{p}' \cdot (\mathbf{p} + \mathbf{r})$  (here we have dropped other terms proportional to  $\mathbf{p} - \mathbf{r}$ ). We rearrange the factor  $(\mathbf{p}' - \mathbf{p})^2 = p_0^2 - (\mathbf{p}' - \mathbf{p})^2$ ; the first term on the rhs causes no difficulty. The second term cancels a photon denominator. Then the integrations over  $\mathbf{p}'$  would give zero by symmetry unless  $\mathbf{p}'$  dependence in  $D_{\mu}(p - p' - r)$  is important. But this happens only for  $|\mathbf{p}'|$  of order  $m_{\mu}$  or greater, in which case  $D_{\mu}(p - p' - r)$  is of order  $m_{\mu}^2$ . The contribution is then of higher order in  $1/m_{\mu}$  than is of present concern.

The product of the electron and muon factors contains a part with the numerator structure

$$[-(p^2 - \gamma^2)\alpha_i\alpha_j + C_{ij}]_e \otimes [-(p^2 - \gamma^2)\alpha_i\alpha_j + C_{ij}]_{\mu} = (p^2 - \gamma^2)^2 \alpha_i\alpha_j \otimes \alpha_i\alpha_j - (p_0^2 + p^2 - \gamma^2)(\alpha_i\alpha_j) \otimes C_{ij} + C_{ij}^e D_{ij}^{\mu}. \tag{B23}$$

For the hfs

$$(\alpha_e \cdot \alpha_{\mu})^2 \doteq -2\sigma_e \cdot \sigma_{\mu}$$

and

$$(\alpha_i\alpha_j) \otimes C_{ij} \doteq \frac{2}{3}\sigma_e \cdot \sigma_{\mu}(3\gamma^2 + \mathbf{p}' \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r} + \mathbf{p}' \cdot \mathbf{r}).$$

Because we wish to reveal similarities and compensations with contributions having different origins, the third term is not analyzed further here. It is decomposed into various pieces in Sec. IV.B.1.

Using (B1), we can rearrange the denominator combinations as follows:

$$\frac{1}{4m_e m_{\mu} D_e(p)} \left[ \frac{1}{D_{\mu}(-p)} - \frac{1}{D_{\mu}(p)} \right] = \frac{1}{8m_e m_{\mu} (m_{\mu}^2 - m_e^2)} \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right] \left[ \frac{E''}{D_e(p)} - \frac{E'}{D_{\mu}(p)} \right]. \tag{B24}$$

In deriving (B24), we have used the fact that the remaining factors in the integrand are even in  $p_0$  and the fact that  $\delta(p_0)/D_e(p) = \delta(p_0)/D_{\mu}(p)$ . The first term of (B23), used most conveniently with the left-hand side of (B24), is treated as the  $[VV]_1$  contribution in Sec. III.E given in (3.21). The remaining terms of (B23) are taken with the right-hand side of (B24) and give the  $[VV]_2$  contribution treated in Sec. IV.B.1 [see (4.14)].

Except for the last two terms in the numerator of (B22d), we have completed our work on the analysis of the algebra of VV. It is not possible to incorporate these remaining terms into VV, since they lead to contributions that do not converge in the intermediate momentum range and cannot be treated independently of VVO and OVV. Here we simply describe how these terms are to be separated into pieces which are to be treated with the two-loop contributions. We can ignore any terms which contain factors of both  $\mathbf{p}'$  and  $\mathbf{r}$ , because they lead to contributions with too many powers of  $\alpha$ . Following the scheme in the discussion of the one-V terms, we identify the terms containing  $\mathbf{r}$ , but not  $\mathbf{p}'$ ,

$$-2\mathbf{r}_j \alpha_{\mu} \cdot \mathbf{p} \alpha_{\mu i} + 2\mathbf{r}_i \alpha_{\mu'}(\mathbf{p} - \mathbf{r})\alpha_{\mu j}, \tag{B25a}$$

which produce the contribution  $(VV)_1$ , and those containing  $\mathbf{p}'$ , but not  $\mathbf{r}$ ,

$$2\mathbf{p}'_j \alpha_{\mu'}(\mathbf{p}' - \mathbf{p})\alpha_{\mu i} + 2\mathbf{p}'_i \alpha_{\mu} \cdot \mathbf{p} \alpha_{\mu j}, \tag{B25b}$$

which produce the contribution  $(VV)_2$ .

To summarize this discussion, we have

$$VV = [VV] + (VV)_1 + (VV)_2 \quad (\text{B26})$$

### b. VVO contribution

Since the treatment follows the same general pattern as previous ones in this appendix, only the main steps are described here. The electron factor is

$$\begin{aligned} EF(\text{VVO}) &= \frac{(E' + m_e + p'_0 + \boldsymbol{\alpha}_e \cdot \mathbf{p}') \alpha_{ei} (E' + \beta_e m_e + p_0 + \boldsymbol{\alpha}_e \cdot \mathbf{p}) \alpha_{ej} (E' + m_e + \boldsymbol{\alpha}_e \cdot \mathbf{r})}{(E' + m_e) D_e(p') D_e(p)} \\ &\doteq \frac{p_0 (2m_e + p'_0) \alpha_{ei} \alpha_{ej}}{D_e(p') D_e(p)} + \frac{(2m_e + p'_0 + \boldsymbol{\alpha}_e \cdot \mathbf{p}') \alpha_{ei} (E' + \beta_e m_e + \boldsymbol{\alpha}_e \cdot \mathbf{p}) \alpha_{ej} (2m_e + \boldsymbol{\alpha}_e \cdot \mathbf{r})}{(E' + m_e) D_e(p') D_e(p)}. \end{aligned} \quad (\text{B27})$$

Next we write out the muon factors, deleting some terms that contain too many powers of  $\alpha$  and non-ln terms that contain too many powers of  $m_e/m_\mu$ :

$$MF(\text{VVO}-1) \doteq \frac{(2m_\mu - p'_0) \alpha_{\mu i} \alpha_{\mu j}}{2m_\mu D_\mu(-p')} - \frac{(p^2 - \gamma^2) \alpha_{\mu i} \alpha_{\mu j}}{D_\mu(-p') D_\mu(-p)} + \frac{(2m_\mu - \boldsymbol{\alpha}_\mu \cdot \mathbf{p}') \alpha_{\mu i} (E'' + \beta_\mu m_\mu - \boldsymbol{\alpha}_\mu \cdot \mathbf{p}) \alpha_{\mu j} (2m_\mu - \boldsymbol{\alpha}_\mu \cdot \mathbf{r})}{2m_\mu D_\mu(-p') D_\mu(-p)}, \quad (\text{B28a})$$

$$MF(\text{VVO}-2) \doteq \frac{\alpha_{\mu i} \alpha_{\mu j}}{4m_\mu^2} + \frac{\alpha_{\mu i} (\mathbf{p}^2 - \boldsymbol{\alpha}_\mu \cdot \mathbf{p}' \boldsymbol{\alpha}_\mu \cdot \mathbf{p}) \alpha_{\mu j}}{D_\mu(p' - p) D_\mu(-p)}, \quad (\text{B28b})$$

$$MF(\text{VVO}-3) \doteq \frac{(2m_\mu + p'_0) \alpha_{\mu i} \alpha_{\mu j}}{2m_\mu D_\mu(p')} + \frac{-(p' - p)^2 \alpha_{\mu i} \alpha_{\mu j} + \alpha_{\mu i} \boldsymbol{\alpha}_\mu \cdot (\mathbf{p}' - \mathbf{p}) \alpha_{\mu j} \boldsymbol{\alpha}_\mu \cdot \mathbf{p}'}{D_\mu(p' - p) D_\mu(p')}, \quad (\text{B28c})$$

$$MF(\text{VVO}-4) \doteq \frac{(2m_\mu - p'_0) \alpha_{\mu j} \alpha_{\mu i}}{2m_\mu D_\mu(-p')} + \frac{E_{ji} - [(p - p' - r)^2 - \gamma^2] \alpha_{\mu j} \alpha_{\mu i}}{D_\mu(-p') D_\mu(p - p' - r)}, \quad (\text{B28d})$$

$$MF(\text{VVO}-5) \doteq \frac{\alpha_{\mu j} \alpha_{\mu i}}{4m_\mu^2} + \frac{\alpha_{\mu j} (\mathbf{p}^2 - \boldsymbol{\alpha}_\mu \cdot \mathbf{p} \boldsymbol{\alpha}_\mu \cdot \mathbf{p}') \alpha_{\mu i}}{D_\mu(p - p') D_\mu(p)}, \quad (\text{B28e})$$

$$MF(\text{VVO}-6) \doteq \frac{(2m_\mu + p'_0) \alpha_{\mu j} \alpha_{\mu i}}{2m_\mu D_\mu(p')} + \frac{-(p^2 - \gamma^2) \alpha_{\mu j} \alpha_{\mu i} + \alpha_{\mu j} \boldsymbol{\alpha}_\mu \cdot \mathbf{p} \alpha_{\mu i} \boldsymbol{\alpha}_\mu \cdot \mathbf{p}'}{D_\mu(p) D_\mu(p')}. \quad (\text{B28f})$$

We first observe that for contributions to the hfs, there are many cancellations between these terms. The first terms of  $MF(1)$  and  $MF(4)$ ,  $MF(2)$  and  $MF(5)$ , and  $MF(3)$  and  $MF(6)$  compensate in this way. The next step is to eliminate all the contributions already incorporated in  $[VV]$ . Also, the contribution corresponding to (B25b) is incorporated into  $[VVO]$  while that of (B25a) is set aside. Having treated the coefficient of  $\delta(p'_0)$ , it is a straightforward matter to expand all the other terms using (B1), keeping only the terms of the order of interest. The result for the product of electron and muon factors is

$$\begin{aligned} \frac{\frac{2}{3} \langle \boldsymbol{\sigma}_e \cdot \boldsymbol{\sigma}_\mu \rangle}{4m_\mu^2 D_e(p') D_e(p)} &\left[ 2[(\mathbf{p} \cdot \mathbf{p}')^2 - \mathbf{p}'^2 \mathbf{p} \cdot \mathbf{p}' - \mathbf{p}^2 \mathbf{p}' \cdot \mathbf{p} + \mathbf{p}^2 \mathbf{p}'^2] \left[ \frac{-2\pi i \delta(p'_0) + 2\pi i \delta(p'_0 - p_0)}{p_0 + i\epsilon} \right] \right. \\ &\left. + 2(\mathbf{p}'^2 + \mathbf{p}' \cdot \mathbf{p}) \mathbf{p}^2 \left[ \frac{-2\pi i \delta(p_0)}{p'_0 + i\epsilon} + \frac{2\pi i \delta(p'_0)}{p_0 + i\epsilon} \right] + 2(\mathbf{p}'^2 - 2\mathbf{p}' \cdot \mathbf{p}) 2\pi i \delta(p'_0) p_0 \right]. \end{aligned} \quad (\text{B29})$$

In summary, the decomposition of VVO is

$$\text{VVO} = [VV] + [VVO] + (VV)_1. \quad (\text{B30})$$

### c. VOV contribution

The electron factor is

$$EF(\text{VOV}) = \frac{(2m_e + \boldsymbol{\alpha}_e \cdot \mathbf{p}'') \alpha_{ei} (E' + \beta_e m_e + p'_0 + \boldsymbol{\alpha}_e \cdot \mathbf{p}') (E' + \beta_e m_e + p_0 + \boldsymbol{\alpha}_e \cdot \mathbf{p}) \alpha_{ej} (2m_e + \boldsymbol{\alpha}_e \cdot \mathbf{r})}{D_e(p') D_e(p)}. \quad (\text{B31})$$

The muon factors for the six graphs are

$$MF(\text{VOV}-1) \doteq \frac{\alpha_{\mu i} \alpha_{\mu j}}{4m_{\mu}^2} + \frac{(\alpha_{\mu} \cdot \mathbf{p}' \alpha_{\mu i} + \alpha_{\mu i} \alpha_{\mu} \cdot \mathbf{p}')(\alpha_{\mu} \cdot \mathbf{p} \alpha_{\mu j} + \alpha_{\mu j} \alpha_{\mu} \cdot \mathbf{r})}{D_{\mu}(-p') D_{\mu}(-p)}, \quad (\text{B32a})$$

$$MF(\text{VOV}-2) \doteq \frac{(2m_{\mu} + p'_0 - p_0) \alpha_{\mu i} \alpha_{\mu j}}{2m_{\mu} D_{\mu}(p' - p)} + \frac{-\alpha_{\mu} \cdot (\mathbf{p}' - \mathbf{p}) \alpha_{\mu i} \alpha_{\mu} \cdot \mathbf{p} \alpha_{\mu j} - p'^2 \alpha_{\mu i} \alpha_{\mu j}}{D_{\mu}(p' - p) D_{\mu}(-p)}, \quad (\text{B32b})$$

$$MF(\text{VOV}-3) \doteq \frac{(2m_{\mu} + p'_0 - p_0) \alpha_{\mu j} \alpha_{\mu i}}{2m_{\mu} D_{\mu}(p' - p)} + \frac{\alpha_{\mu} \cdot (\mathbf{p}' - \mathbf{p}) \alpha_{\mu j} \alpha_{\mu} \cdot \mathbf{p}' \alpha_{\mu i} - p'^2 \alpha_{\mu j} \alpha_{\mu i}}{D_{\mu}(p' - p) D_{\mu}(p')}, \quad (\text{B32c})$$

$$MF(\text{VOV}-4) \doteq \frac{(2m_{\mu} + p_0 - p'_0) \alpha_{\mu i} \alpha_{\mu j}}{2m_{\mu} D_{\mu}(p - p')} + \frac{-\alpha_{\mu i} \alpha_{\mu} \cdot \mathbf{p}' \alpha_{\mu j} \alpha_{\mu} \cdot (\mathbf{p} - \mathbf{p}') - p'^2 \alpha_{\mu i} \alpha_{\mu j}}{D_{\mu}(-p') D_{\mu}(p - p')}, \quad (\text{B32d})$$

$$MF(\text{VOV}-5) \doteq \frac{(2m_{\mu} + p_0 - p'_0) \alpha_{\mu j} \alpha_{\mu i}}{2m_{\mu} D_{\mu}(p - p')} + \frac{\alpha_{\mu j} \alpha_{\mu} \cdot \mathbf{p} \alpha_{\mu i} \alpha_{\mu} \cdot (\mathbf{p} - \mathbf{p}') - p'^2 \alpha_{\mu j} \alpha_{\mu i}}{D_{\mu}(p) D_{\mu}(p - p')}, \quad (\text{B32e})$$

$$MF(\text{VOV}-6) \doteq \frac{\alpha_{\mu j} \alpha_{\mu i}}{4m_{\mu}^2} + \frac{\alpha_{\mu j} \alpha_{\mu} \cdot \mathbf{p} \alpha_{\mu} \cdot \mathbf{p}' \alpha_{\mu i}}{D_{\mu}(p') D_{\mu}(p)}. \quad (\text{B32f})$$

Here we have dropped terms of higher order in  $\alpha$  or in  $m_e/m_{\mu}$ . As in the case of VVO, we note a pairwise cancellation of the first terms of these expressions for the contribution to the hfs.

We shall concentrate on Caswell-Lepage pairs in (B32) [(B32a) and (B32f), (B32b) and (B32e), and (B32c) and (B32d)]. These have the property that the leading terms cancel in the intermediate momentum range. (Recall that to determine the hfs content of an expression, we can reverse the order of its  $\alpha$  matrices and change its sign.) In each term, we use (B1a) to rearrange the muon denominators. External momenta are important only in combination with two loop-energy  $\delta$  functions. Terms not involving external momenta would be logarithmically divergent were it not for the Caswell-Lepage cancellation. This implies that they must be treated with care; the mere appearance of a factor of  $m_{\mu}$  in a denominator does not in itself guarantee that an integral is negligible. Taking into account the Caswell-Lepage cancellation, we need keep only the first term of (B1a) in every case as far as high-momentum convergence is concerned. The only possible difficulty is that there may be a low-momentum singularity which might lead to  $\ln \alpha$ . Careful investigation shows that this does not happen. One disadvantage of this approach is that the argument of the logarithm is not treated symmetrically, as in previous cases.

The result for the sum of terms is

$$MF(\text{VOV}) = \frac{(\alpha_{\mu} \cdot \mathbf{p}' \alpha_{\mu i} + \alpha_{\mu i} \alpha_{\mu} \cdot \mathbf{p}')(\alpha_{\mu} \cdot \mathbf{p} \alpha_{\mu j} + \alpha_{\mu j} \alpha_{\mu} \cdot \mathbf{r})}{4E^2} \left[ (-2\pi i)^2 \delta(p_0) \delta(p'_0) + \frac{2\pi i \delta(p_0)}{p'_0 + i\epsilon} + \frac{2\pi i \delta(p'_0)}{p_0 + i\epsilon} \right] \\ - \frac{\alpha_{\mu} \cdot (\mathbf{p}' - \mathbf{p}) \alpha_{\mu i} \alpha_{\mu} \cdot \mathbf{p} \alpha_{\mu j} + p'^2 \alpha_{\mu i} \alpha_{\mu j}}{4m_{\mu}^2} \left[ \frac{-2\pi i \delta(p_0) + 2\pi i \delta(p'_0 - p_0)}{p'_0 + i\epsilon} \right] \\ - \frac{\alpha_{\mu i} \alpha_{\mu} \cdot \mathbf{p}' \alpha_{\mu j} \alpha_{\mu} \cdot (\mathbf{p} - \mathbf{p}') + p'^2 \alpha_{\mu i} \alpha_{\mu j}}{4m_{\mu}^2} \left[ \frac{-2\pi i \delta(p'_0) + 2\pi i \delta(p'_0 - p_0)}{p_0 + i\epsilon} \right]. \quad (\text{B33})$$

The reader should note that the Caswell-Lepage cancellation is satisfied for (B33). This result is used in Sec. IV.B.3.

The complete two-V result is

$$\text{VVO} + \text{VOV} + \text{OVV} = [\text{VV}] + [\text{VVO}] + [\text{VOV}] + [\text{OVV}]. \quad (\text{B34})$$

### 3. Pure-O contribution

According to Sec. III.B, the quantity to be analyzed is  $\text{OOO} - \text{OO}$ , with small muon components incorporated into the wave function. However, the effects of those small components cancel between  $\text{OOO}$  and  $-\text{OO}$  to the order of interest. Therefore, we shift our attention to  $\text{OOO}$  with the small components dropped. Then it is also easy to see that the small electron components do not contribute to the hfs to the order of interest (one considers the appropriate integral and uses symmetry). The contribution to the hfs is then easily seen to be given by

$$\frac{\alpha_e \cdot \mathbf{p}' \alpha_e \cdot \mathbf{p} \alpha_\mu \cdot \mathbf{p}' \alpha_\mu \cdot \mathbf{p}}{D_e(p') D_e(p)} \left[ \frac{1}{D_\mu(-p') D_\mu(-p)} - \frac{1}{D_\mu(p') D_\mu(p)} - \frac{1}{D_\mu(-p') D_\mu(p-p')} \right. \\ \left. + \frac{1}{D_\mu(p') D_\mu(p'-p)} + \frac{1}{D_\mu(p) D_\mu(p-p')} - \frac{1}{D_\mu(-p) D_\mu(p'-p)} \right]. \quad (\text{B35})$$

The terms have been arranged so that each successive pair provides a Caswell-Lepage cancellation. To see this, one may neglect the  $E'$  in  $D_e$  and reverse the signs of  $p$  and  $p'$  in one of the terms of the pair.

The next step is to use (B1a) for all the muon denominators. We argue that only the first terms need be kept for muonium. The reason is that they turn out to satisfy the Caswell-Lepage cancellation separately, and the terms dropped have no sensitivity to small photon momenta which could lead to  $\ln\alpha$  contributions. The resulting expression is relatively simple:

$$\frac{\alpha_e \cdot \mathbf{p}' \alpha_e \cdot \mathbf{p} \alpha_\mu \cdot \mathbf{p}' \alpha_\mu \cdot \mathbf{p}}{4E^2 D_e(p') D_e(p)} \left[ (2\pi i)^2 \delta(p'_0) \delta(p_0) + \frac{4\pi i \delta(p'_0)}{p_0 + i\epsilon} + \frac{4\pi i \delta(p_0)}{p'_0 + i\epsilon} - \frac{4\pi i \delta(p'_0 - p_0)}{p_0 + i\epsilon} \right]. \quad (\text{B36})$$

This expression is used in Sec. IV.C.

#### 4. Three-V contribution

Unlike previous contributions, this one has no associated subtractions. Also, to the order of interest, small components of the wave function can be ignored. The electron factor is found to be

$$EF(\text{VVV}) \doteq \frac{\alpha_{ei}(p'_0 \alpha_{ej} \alpha_e \cdot \mathbf{p} + \alpha_e \cdot \mathbf{p}' \alpha_{ej} p_0) \alpha_{ek}}{D_e(p') D_e(p)}. \quad (\text{B37})$$

The muon factor, arranged in Caswell-Lepage pairs is

$$MF(\text{VVV}) \doteq \alpha_{\mu i}(p'_0 \alpha_{\mu j} \alpha_\mu \cdot \mathbf{p} + \alpha_\mu \cdot \mathbf{p}' \alpha_{\mu j} p_0) \alpha_{\mu k} \left[ \frac{1}{D_\mu(-p') D_\mu(-p)} - \frac{1}{D_\mu(p') D_\mu(p)} \right] \\ + \alpha_{\mu i} [p'_0 \alpha_{\mu k} \alpha_\mu \cdot (\mathbf{p}' - \mathbf{p}) + \alpha_\mu \cdot \mathbf{p}' \alpha_{\mu k} (p'_0 - p_0)] \alpha_{\mu j} \left[ \frac{1}{D_\mu(-p') D_\mu(p-p')} - \frac{1}{D_\mu(p') D_\mu(p'-p)} \right] \\ + \alpha_{\mu j} [\alpha_\mu \cdot (\mathbf{p} - \mathbf{p}') \alpha_{\mu i} p_0 + (p_0 - p'_0) \alpha_{\mu i} \alpha_\mu \cdot \mathbf{p}] \alpha_{\mu k} \left[ \frac{1}{D_\mu(-p) D_\mu(p'-p)} - \frac{1}{D_\mu(p) D_\mu(p-p')} \right]. \quad (\text{B38})$$

Next we use (B1a), retaining only the first terms. Because of the Caswell-Lepage cancellation, any contributions involving the second terms are negligible for muonium; also, they have no low-momentum sensitivity which could produce  $\ln\alpha$  contributions. Finally we take the product of the spin factors and use angular averaging of the integration to simplify the result. Note also that  $(\sigma_e \cdot \sigma_\mu)^2 \doteq -2(\sigma_e \cdot \sigma_\mu)$  and  $(\sigma_e \cdot \sigma_\mu)^4 \doteq -20(\sigma_e \cdot \sigma_\mu)$  for purposes of the hfs. Then we find for the product of the electron and muon factors

$$\frac{\frac{2}{3} \langle \sigma_e \cdot \sigma_\mu \rangle [-2\pi i \delta(p_0) 6p'_0 \mathbf{p}^2 - 2\pi i \delta(p'_0) 6p_0 \mathbf{p}'^2 + 2\pi i \delta(p_0 - p'_0) 2p_0 (\mathbf{p} - \mathbf{p}')^2]}{4E^2 D_e(p') D_e(p)}. \quad (\text{B39})$$

This result is used in Sec. IV.D.

### APPENDIX C: CALCULATION OF INTEGRALS

In this appendix we describe the calculation of the various two-, three-, and four-loop integrals mentioned in the body of the text and tabulate the results of those calculations. In each case, we retain only the leading power of  $\gamma$  in the result. This permits us to develop special tricks which make possible analytic calculation of the two-loop integrals. Since the three- and four-loop integrals are homogeneous in  $\gamma$ , the results we report for them are exact.

#### 1. Two-loop integrals

The two-loop integrals are of the form

$$K_i = (4\pi)^2 \int \frac{d^4 p' d^4 p}{-(2\pi)^8} \frac{G_i(p'_0, p_0, m) P(\mathbf{p}', \mathbf{p}, \gamma)}{(p'^2 - \gamma^2 + i\epsilon) D(p') [(p-p')^2 + i\epsilon] D(p) (p^2 - \gamma^2 + i\epsilon)}. \quad (\text{C1})$$

Here  $D(p) = 2mp_0 + p^2 - \gamma^2 + i\epsilon$ ,  $P$  is a polynomial that is an invariant in the spatial momenta (up to quartic terms) and can contain even powers of  $\gamma$ , and  $G_i$  contains at least one  $\delta$  function involving the time components of momenta and in some cases it contains a factor of  $m$ . The factors  $G_i$  and  $P$  always appear in combinations such that the total integral is dimensionless. The integrals are structured so as to reflect the Caswell-Lepage cancellation—i.e., for momenta large compared to  $m$  (which may be  $m_e$  or  $m_\mu$ ) symmetric integration guarantees the convergence of the integral. In some cases, it is convenient to separate different terms in the integrand by introducing some temporary regulator (for example, dimensional regularization).

The integrals separate into several broad groups, each of which is treated somewhat differently. In the first group ( $K_1$  to  $K_6$ ), the function  $G$  has degree  $-2$  and the polynomial  $P$  has degree  $+4$ . In the second group ( $K_7$  to  $K_9$ ),  $G$  has degree  $0$  and  $P$  has degree  $2$ .  $K_{10}$  is an individual integral in which the degree of  $G$  is  $+2$  and  $P$  is a constant. For the third group ( $K_{11}$  to  $K_{13}$ ),  $G$  has degree  $-1$  in the loop energy but also has a power of  $m$  in the numerator; the polynomial  $P$  then has degree  $+2$ . Finally, there are two types of integrals ( $K_{14}$  and  $K_{15}$ ) in which  $G$  has degree  $-3$  in the energy and a factor of  $m$ , while  $P$  is of degree  $+4$ . This last group is particularly delicate, since it contains spurious low-momentum divergences that cancel only for certain combinations of numerator terms. The different forms of  $G$  are given in Table III.

For cases in which  $P$  contains  $\gamma^2$  or  $\gamma^4$ , we can obtain the contribution of order of interest (i.e.,  $\gamma^0$ ) only if the integral produces inverse powers of  $\gamma$ . In all these cases, we can get a contribution only if the integrand has a factor  $\delta(p'_0)\delta(p_0)$ . This factor may be present in terms in  $G$ , or it may arise from use of the approximation (3.10) on the denominators  $D$ . With the double  $\delta$ -function structure, we have an integral over spatial momenta only. It can be evaluated by Fourier transforming to coordinate space, and the resulting three-dimensional integral consists of elementary forms.

Next let us take up the case in which  $P$  is a polynomial in the spatial momenta only. Our general strategy for evaluating these integrals is as follows. First we use Feynman parameters to combine denominators and carry out the spatial momentum integrations in the standard way, using analytic regularization to make various pieces of the integral converge separately. In carrying out the  $p_0$  and  $p'_0$  integration, we retain only contributions with the leading power of  $\gamma$ , some of which have  $\ln\gamma$  dependence. We find that the leading contribution generally has a much simpler parameter integral dependence than the complete integral. We are then able to construct integrals

TABLE III. Various categories of integrals defined by  $G_i(p'_0, p_0, m)$ .

|          | $G_i$   |
|----------|---|
| $K_1$    | $-2\pi i \delta(p'_0) \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right]$         |
| $K_2$    | $-2\pi i \delta(p_0) \left[ -2\pi i \delta(p'_0) - \frac{2}{p'_0 + i\epsilon} \right]$        |
| $K_3$    | $-2\pi i \delta(p_0 - p'_0) \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right]$   |
| $K_4$    | $\frac{-2\pi i \delta(p_0)}{p'_0 + i\epsilon} - \frac{-2\pi i \delta(p'_0)}{p_0 + i\epsilon}$ |
| $K_5$    | $\frac{-2\pi i \delta(p_0) + 2\pi i \delta(p_0 - p'_0)}{p'_0 + i\epsilon}$                    |
| $K_6$    | $\frac{-2\pi i \delta(p'_0) + 2\pi i \delta(p_0 - p'_0)}{p_0 + i\epsilon}$                    |
| $K_7$    | $-2\pi i \delta(p'_0) p_0$  |
| $K_8$    | $-2\pi i \delta(p_0) p'_0$  |
| $K_9$    | $-2\pi i \delta(p_0 - p'_0) p_0$  |
| $K_{10}$ | $-2\pi i \delta(p_0 - p'_0) p_0^3$  |
| $K_{11}$ | $-2\pi i \delta(p_0 - p'_0) 2m$   |
| $K_{12}$ | $-2\pi i \delta(p_0) 2m$  |
| $K_{13}$ | $-2\pi i \delta(p'_0) 2m$   |
| $K_{14}$ | $\frac{-2\pi i \delta(p_0 - p'_0) 2m}{(p_0 + i\epsilon)^2}$                                   |
| $K_{15}$ | $\frac{-2\pi i \delta(p_0) 2m}{(p'_0 + i\epsilon)^2}$   |

involving only the six spatial momenta which yield the same parameter integral. These six-dimensional integrals can be evaluated straightforwardly by Fourier transforming to coordinate space, where they ultimately become one-dimensional integrals.

Before we discovered the method just described, the most natural one seemed to be one in which the loop energy integrations were carried out first, using the method of residues. However, this led to expressions in which there are delicate cancellations between terms and which are so complicated that there was no hope of carrying out the subsequent spatial momenta integrals analytically. Such integrals can be worked out numerically, of course, and most of the integrals presented here have been checked that way to a few percent accuracy.

In order to illustrate this procedure, we work through some typical integrals in detail. We first take the cases

$$G_7 = -2\pi i p_0 \delta(p'_0), \quad P = \mathbf{p}^2 \text{ or } \mathbf{p} \cdot \mathbf{p}'. \quad (C2)$$

After combining denominators, we find that the required integral is

$$K_7(\mathbf{p}^2; \mathbf{p} \cdot \mathbf{p}') = \lim_{\lambda \rightarrow 5} (4\pi)^2 \int_{-\infty}^{\infty} \frac{p_0 dp_0}{-2\pi i} \frac{d^3 p d^3 p'}{(2\pi)^6} \int_0^1 (dx) \frac{4\{\mathbf{p}^2; \mathbf{p} \cdot \mathbf{p}'\}}{(-dp_0^2 - 2emp_0 + a\mathbf{p}^2 - 2b\mathbf{p} \cdot \mathbf{p}' + c\mathbf{p}'^2 + f\gamma^2 - i\epsilon)^\lambda}, \quad (C3)$$

where

$$(dx) = \prod_{i=1}^4 dx_i \delta \left[ 1 - \sum_{i=1}^4 x_i \right],$$

$a, \dots, f$  are sums of certain of the  $x_i$ , and  $\lambda$  is the analytic regularization parameter.

Note that the only polynomials which occur in  $K_7$  have a factor of  $\mathbf{p}'$ . Examination of the original integral shows that if such a factor were not present (e.g., if the polynomial were  $\mathbf{p}^2$  or  $\gamma^2$ ), we could not simply let  $\gamma \rightarrow 0$  in the denominator without producing a low-momentum divergence in the loop containing  $\mathbf{p}'$ . Taking the denominator  $\gamma$  dependence into account, we find the subintegral would give a factor  $\gamma^{-1}$ . Thus the result can be neglected for the  $\gamma^2$  numerator, but it would give a spurious lower-order term for the  $\mathbf{p}^2$  numerator. We have not tried to work this out, but estimate that it would have the structure  $\alpha^{-1} \ln \alpha$ . One of the subtleties of our treatment, which is sometimes hidden from the reader, is that occasionally such spurious terms pop up when the calculational path is followed too mechanically, and related contributions are allowed to become separated because they seemingly arise from different contexts.

The integration over the spatial momenta yields

$$K_7(\mathbf{p}'^2; \mathbf{p} \cdot \mathbf{p}') = \lim_{\lambda \rightarrow 5} \int_{-\infty}^{\infty} \frac{p_0 dp_0}{-2\pi i} \frac{1}{4\pi} \int_0^1 \frac{(dx)}{(ac - b^2)^{5/2}} \frac{\frac{3}{2} 4! \{a; b\} \Gamma(\lambda - 4) / \Gamma(\lambda)}{(-dp_0^2 - 2emp_0 + f\gamma^2 - i\epsilon)^{\lambda - 4}}. \quad (C4)$$

To obtain the leading contribution, we can safely drop the  $f\gamma^2$  term in the denominator. Then the  $p_0$  integration yields

$$K_7(\mathbf{p}'^2; \mathbf{p} \cdot \mathbf{p}') = \frac{1}{4\pi} \int_0^1 (dx) \frac{\frac{3}{4} \{a; b\}}{d(ac - b^2)^{5/2}}. \quad (C5)$$

(Note that a potential logarithmic divergence has cancelled by symmetry.)

The  $a$  and  $b$  dependence of (B5) arises solely from the structure of the  $\mathbf{p}'$  and  $\mathbf{p}$  dependence of the numerator and denominator. The factor of  $d$  in the denominator is simply the sum of parameters of the denominators which contain  $-p_0^2$ . It turns out that there is another way to arrive at a similar result from a different integral. Consider an integral involving spatial moment only [i.e., replace  $G_7$  by  $(-2\pi i)^2 \delta(p_0') \delta(p_0)$ ], but keep the same numerator and denominator dependence on  $\mathbf{p}'$  and  $\mathbf{p}$ . Also, drop the  $\gamma^2$  in the denominators, and introduce a term  $+\rho^2$  in each denominator that originally contained a term  $-p_0^2$ . The result can be inferred from (C4) to be

$$K_7(\mathbf{p}'^2; \mathbf{p} \cdot \mathbf{p}') = \frac{1}{4\pi} \int_0^1 (dx) \frac{\frac{3}{2} \{a; b\}}{(ac - b^2)^{5/2} d\rho^2}. \quad (C6)$$

Thus we can immediately write down an integral over spatial momentum which reproduces our *approximate* result for (C3):

$$K_7(\mathbf{p}'^2; \mathbf{p} \cdot \mathbf{p}') \doteq - (4\pi)^2 \frac{\rho^2}{2} \int \frac{d^3 p' d^3 p}{(2\pi)^6} \frac{\{\mathbf{p}'^2; \mathbf{p} \cdot \mathbf{p}'\}}{\mathbf{p}'^2 \mathbf{p}'^2 [(\mathbf{p}' - \mathbf{p})^2 + \rho^2] (\mathbf{p}^2 + \rho^2) (\mathbf{p}^2 + \rho^2)}. \quad (C7)$$

(Note again the difficulty if there were no factor of  $\mathbf{p}'$  in the numerator.) Fourier transforming this to coordinate space, we obtain

$$\begin{aligned} K_7(\mathbf{p}'^2; \mathbf{p} \cdot \mathbf{p}') &\doteq - \frac{\rho^2}{2} \int_0^\infty dr r^2 \left\{ \frac{1}{r}; \frac{\rho}{2} \right\} \frac{e^{-\rho r}}{r} \frac{e^{-\rho r}}{2\rho} \\ &= \left\{ -\frac{1}{8}; -\frac{1}{32} \right\}. \end{aligned} \quad (C8)$$

These results, and other ones from integrals of the same type, are contained in Table V.

Next let us consider a somewhat more complicated example that leads to a result containing  $\ln(m/\gamma)$ :

$$G_1 = -2\pi i \delta(p_0') \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right], \quad (C9)$$

$$P = \mathbf{p}^2 \mathbf{p}'^2; \mathbf{p} \cdot \mathbf{p}' \mathbf{p}'^2; \mathbf{p} \cdot \mathbf{p}' \mathbf{p}^2; (\mathbf{p}' \cdot \mathbf{p})^2.$$

After we combine denominators, the integration over the spatial components of momenta gives

$$K_1 = \lim_{\lambda \rightarrow 5} \int_{-\infty}^{\infty} \frac{dp_0}{-2\pi i} \left[ -2\pi i \delta(p_0) - \frac{2}{p_0 + i\epsilon} \right] \frac{4!}{4\pi} \frac{\Gamma(\lambda - 5)}{\Gamma(\lambda)} \int_0^1 (dx) \frac{Q(a, b, c)}{(ac - b^2)^{7/2} (-dp_0^2 - 2emp_0 + f\gamma^2)^{\lambda - 5}}, \quad (C10)$$

where  $Q$  is a quadratic form in  $a, b, c$  which depends on the choice of  $P$ . For the  $\delta(p_0)$  term, the  $p_0$  integration gives



TABLE IV. Results of the integrations for  $K_1$  through  $K_6$  for different polynomials.

|       | $\mathbf{p}^2\mathbf{p}'^2$             | $\mathbf{p}^2\mathbf{p}\cdot\mathbf{p}'$                  | $\mathbf{p}'^2\mathbf{p}\cdot\mathbf{p}'$                 | $(\mathbf{p}'\cdot\mathbf{p})^2$                          |
|-------|---|---|---|---|
| $K_1$ | $-\ln\frac{m}{2\gamma} + \frac{11}{16}$ | $-\frac{1}{2}\ln\frac{m}{2\gamma} + \frac{5}{8}$          | $-\frac{1}{2}\ln\frac{m}{2\gamma} + \frac{5}{16}$         | $-\frac{1}{2}\ln\frac{m}{2\gamma} + \frac{7}{16}$         |
| $K_2$ | $-\ln\frac{m}{2\gamma} + \frac{11}{16}$ | $-\frac{1}{2}\ln\frac{m}{2\gamma} + \frac{5}{16}$         | $-\frac{1}{2}\ln\frac{m}{2\gamma} + \frac{5}{8}$          | $-\frac{1}{2}\ln\frac{m}{2\gamma} + \frac{7}{16}$         |
| $K_3$ | $-\ln\frac{m}{2\gamma} + \frac{7}{8}$   | $-\frac{1}{2}\ln\frac{m}{2\gamma} - 2\ln 2 + \frac{9}{8}$ | $-\frac{1}{2}\ln\frac{m}{2\gamma} - 2\ln 2 + \frac{9}{8}$ | $-\frac{1}{2}\ln\frac{m}{2\gamma} - 2\ln 2 + \frac{9}{8}$ |
| $K_4$ | 0                                       | $\frac{5}{32}$  | $-\frac{5}{32}$   | 0   |
| $K_5$ | $-\ln 2 + \frac{3}{32}$                 | $-\ln 2 + \frac{13}{32}$                                  | $-\ln 2 + \frac{1}{4}$                                    | $-\ln 2 + \frac{11}{32}$                                  |
| $K_6$ | $-\ln 2 + \frac{3}{32}$                 | $-\ln 2 + \frac{1}{4}$                                    | $-\ln 2 + \frac{13}{32}$                                  | $-\ln 2 + \frac{11}{32}$                                  |

|                 | $\mathbf{p}^2\gamma^2$ | $\mathbf{p}'^2\gamma^2$ | $\mathbf{p}\cdot\mathbf{p}'\gamma^2$ | $\gamma^4$      |
|-----------------|------------------------|-------------------------|--------------------------------------|-----------------|
| $K_1, K_2, K_3$ | $-\frac{3}{16}$        | $-\frac{3}{16}$         | $-\frac{1}{16}$                      | $-\frac{1}{16}$ |
| $K_4, K_5, K_6$ | 0                      | 0                       | 0                                    | 0               |

$$K_1^{(1)} = \lim_{\lambda \rightarrow 5} \frac{4!}{4\pi} \frac{\Gamma(\lambda-5)}{\Gamma(\lambda)} \int_0^1 (dx) \frac{Q(a,b,c)}{(ac-b^2)^{7/2} (f\gamma^2)^{\lambda-5}} \tag{C11a}$$

For the  $2/(p_0 + i\epsilon)$  term, we can neglect  $f\gamma^2$  in the denominator. Then the  $p_0$  integration gives

$$K_1^{(2)} = -\lim_{\lambda \rightarrow 5} \frac{4!}{4\pi} \frac{\Gamma(\lambda-5)}{\Gamma(\lambda)} \frac{1}{\pi^{1/2}} \frac{\Gamma(\lambda-\frac{9}{2})}{\Gamma(\lambda-4)} \int_0^1 (dx) \frac{Q(a,b,c)}{(ac-b^2)^{7/2} \left[ \frac{e^2 m}{d} \right]^{\lambda-5}} \tag{C11b}$$

Note that the two expressions (C11a) and (C11b) separately contain poles as  $\lambda \rightarrow 5$  arising from  $\Gamma(\lambda-5) = \Gamma(\lambda-4)/(\lambda-5)$ , but that this singularity cancels in the sum. In the vicinity of the pole, we expand other factors in powers of  $\lambda-5$  (e.g.,  $\Gamma(\lambda-\frac{9}{2})/\Gamma(\lambda-4) \approx \pi^{1/2}[1 - (\lambda-5)\ln 4]$ ). After cancellation of the pole terms, we are left with

$$K_1 = \frac{-1}{4\pi} \int_0^1 (dx) \frac{Q(a,b,c) \ln \frac{fd\gamma^2}{4e^2 m^2}}{(ac-b^2)^{7/2}} \tag{C12}$$

We rewrite the argument of the ln as  $(f\gamma^2)(d\rho^2)/(e4m^2)(e\rho^2)$ . Each of the factors in the argument can now be associated with an (analytically regulated) integral over spatial momenta only, the divergence cancelling in the sum. At this stage, the result can be reexpressed:

TABLE V. Results of the integrations for  $K_7$  through  $K_{13}$  for different polynomials.

|          | $\mathbf{p}'^2$                                 | $\mathbf{p}\cdot\mathbf{p}'$                    | $\mathbf{p}^2$                                  | $\gamma^2$    |
|----------|---|---|---|---------------|
| $K_7$    | $-\frac{1}{8}$                                  | $-\frac{1}{32}$                                 |   | 0             |
| $K_8$    |   | $-\frac{1}{32}$                                 | $-\frac{1}{8}$                                  | 0             |
| $K_9$    | $-\frac{3}{32}$                                 | $-\frac{1}{32}$                                 | $-\frac{3}{32}$                                 | 0             |
| $K_{11}$ | ln2   | $\ln 2 - \frac{1}{2}$                           | ln2   | 0             |
| $K_{12}$ |   | $\frac{1}{4}\ln\frac{m}{2\gamma} - \frac{1}{4}$ | $\frac{1}{2}\ln\frac{m}{2\gamma} - \frac{1}{8}$ | $\frac{1}{8}$ |
| $K_{13}$ | $\frac{1}{2}\ln\frac{m}{2\gamma} - \frac{1}{8}$ | $\frac{1}{4}\ln\frac{m}{2\gamma} - \frac{1}{4}$ |   | $\frac{1}{8}$ |

$$K_{10} = \frac{1}{32}$$

$$K_1 = (4\pi)^2 \int \frac{d^3p'd^3p}{(2\pi)^6} \left[ \frac{-1}{(\mathbf{p}'^2 + \gamma^2)^2 (\mathbf{p}' - \mathbf{p})^2 (\mathbf{p}^2 + \gamma^2)^2} + \frac{1}{(\mathbf{p}'^2)^2 (\mathbf{p}' - \mathbf{p})^2 \mathbf{p}^2 (\mathbf{p}^2 + 4m^2)} \right. \\ \left. + \frac{1}{(\mathbf{p}'^2)^2 (\mathbf{p}' - \mathbf{p})^2 \mathbf{p}^2 (\mathbf{p}^2 + \rho^2)} - \frac{1}{(\mathbf{p}'^2)^2 [(\mathbf{p}' - \mathbf{p})^2 + \rho^2] (\mathbf{p}^2 + \rho^2)^2} \right] P. \quad (\text{C13})$$

In the Fourier transformation to coordinate space, it is useful to write the numerator factors of momenta in  $P$  as derivatives with respect to the coordinate space variables. The resulting three-dimensional integral is tedious, but straightforward to evaluate. The results are presented in Table IV below.

The other two-loop integrals can be evaluated by using similar techniques. However, for some of them a few additional tricks are required. In  $K_{12}$  and  $K_{13}$  the integration over momentum variables results in an expression proportional to  $(e^2 m^2 + f d \gamma^2)^{-1/2}$ . It is tempting at this stage to neglect the term proportional to  $\gamma^2$ , as we did in the previous examples. However, in these integrals  $e$  consists of a single Feynman parameter, so the result would diverge. We get around this problem by first using the method of partial fractions to rearrange the original integrand. For  $K_{12}$  we use

$$\frac{1}{p'^2 - \gamma^2 + i\epsilon} \frac{1}{D(p')} = \frac{1}{2m(p'_0 + i\epsilon)} \left[ \frac{1}{p'^2 - \gamma^2 + i\epsilon} - \frac{1}{D(p')} \right]. \quad (\text{C14})$$

For  $K_{13}$  we replace  $p'$  by  $p$  in this expression. Now the integral has only four denominators which are quadratic forms in the momenta, so it is again useful to use analytic regularization. With the rearrangement, the parameter  $e$  winds up as the argument of a logarithm, so the parameter integration is convergent. We can then follow the previously developed procedure. It is not surprising that the final result contains terms of the form  $\ln(m/\gamma)$  which were signaled by the original structure of the parameter integral.

The  $K_{14}$  and  $K_{15}$  integrals are the most subtle ones. The result of the integration over the momentum variables is proportional to

$$\left[ \frac{em}{d} + \left[ \frac{e^2 m^2}{d^2} + \frac{f \gamma^2}{d} \right]^{1/2} \right]^{-1}.$$

For  $K_{14}$ ,  $e$  consists of a sum of two Feynman parameters, so we can neglect the term proportional to  $\gamma^2$ . The result of this step is proportional to  $d/em$ . Now we want to obtain the same structure from an integration over spatial momenta only. To obtain the numerator factor of  $d$ , we start with an expression containing the usual five denominators, which are combined with Feynman parameters. We add a quantity  $\sigma$  to each denominator that originally contained a term  $-p_0^2$ . Then we simply differentiate the expression with respect to  $\sigma$  and set  $\sigma=0$ . The factor  $1/e$  can be obtained by using the trick employed for  $K_7$ : we add a term  $\rho^2$  to each denominator that originally contained a term  $-2mp_0$ . Thus we express the result as a spatial momentum integral which can be converted to a coordinate space integral.

For  $K_{15}$ ,  $e$  consists of a single Feynman parameter, so we first use the partial fractions trick (C14). Then it is convenient to transform it further by integrating by parts with respect to  $p'_0$ . At this stage the various pieces of the integrand take the form of integrals which we have already discussed. The numerator structures for  $P$  are chosen so as to cancel some spurious divergences.

The results for all the two-loop integrals are tabulated in Tables III–VIII. Note that the integrals are well defined only as analytically regulated expressions, since they contain logarithmic divergences which cancel by symmetry.

## 2. Three- and four-loop integrals

Now let us discuss the three-loop and four-loop integrals used in the main text. These are

$$I_1 = \int d^3p'd^3p d^3r \frac{\mathbf{p}' \cdot \mathbf{r}}{(\mathbf{p}'^2 + \gamma^2)^2 (\mathbf{p}' - \mathbf{p})^2 (\mathbf{p} - \mathbf{r})^2 (\mathbf{r}^2 + \gamma^2)^2}, \quad (\text{C15a})$$

$$I_2 = \int d^3p'd^3p d^3r \frac{[(\mathbf{p}' - \mathbf{p}) \cdot (\mathbf{p} - \mathbf{r})]^2 - [\mathbf{p}' \cdot (\mathbf{p}' - \mathbf{p})]^2 - [\mathbf{p}' \cdot (\mathbf{p} - \mathbf{r})]^2 + (\mathbf{p}^2)^2}{(\mathbf{p}'^2 + \gamma^2)^2 (\mathbf{p}' - \mathbf{p})^2 (\mathbf{p}^2 + \gamma^2)^2 (\mathbf{p} - \mathbf{r})^2 (\mathbf{r}^2 + \gamma^2)^2}, \quad (\text{C15b})$$

and

$$I_3 = \int d^3p'' d^3p' d^3p d^3r \frac{[(\mathbf{p}'' - \mathbf{p}') \cdot (\mathbf{p} - \mathbf{r})]^2 - (\mathbf{p}' \cdot \mathbf{p})^2}{(\mathbf{p}''^2 + \gamma^2)^2 (\mathbf{p}'' - \mathbf{p}')^2 (\mathbf{p}'^2 + \gamma^2)^2 (\mathbf{p}' - \mathbf{p})^2 (\mathbf{p}^2 + \gamma^2)^2 (\mathbf{p} - \mathbf{r})^2 (\mathbf{r}^2 + \gamma^2)^2}. \quad (\text{C15c})$$

$I_1$  is easily evaluated by Fourier transforming to coordinate space. Since the integrand contains no denominators involving  $\mathbf{p}^2$ , the coordinate space integral is only three dimensional and is very similar in structure to the integrals that arose in the two loop case. We merely report the result in Table VIII below.

In the three-loop integral  $I_2$  and the four-loop integral  $I_3$ , the individual terms lead to divergent expressions, so it is important to manipulate the integrand as a whole. We make use of an approach similar to the one employed in the second-order perturbation calculation of Sec. V. First we Fourier transform with respect to the variables  $\mathbf{p}'$ ,  $\mathbf{p}' - \mathbf{p}$ ,  $\mathbf{p} - \mathbf{r}$ ,  $\mathbf{r}$  in  $I_2$ ;  $I_3$  is treated in an analogous manner. The denominator  $\mathbf{p}^2 + \gamma^2$  and the numerator momentum factors become differential operators acting on the coordinate space factors that arise from the denominators  $(\mathbf{p}'^2 + \gamma^2)^2$ ,  $(\mathbf{p}' - \mathbf{p})^2$ ,  $(\mathbf{p} - \mathbf{r})^2$ , and  $(\mathbf{r}^2 + \gamma^2)^2$ . (Note that the denominators  $\mathbf{p}^2 + \gamma^2$  are essentially nonlocal operators.) Since in each integral the number of (three-dimensional) coordinate space variables is just one more than the number of (three-dimensional) momentum variables, the resulting coordinate space integral is three-dimensional. In evaluating the coordinate space integrals, it is convenient to resolve factors into their (orthogonal)  $S$ - and  $D$ -wave parts, as in Sec. V.

The required Fourier transforms are

$$\frac{1}{(\mathbf{p}^2 + \gamma^2)^2} \rightarrow \frac{\pi^2}{\gamma} e^{-\gamma r} \tag{C16a}$$

and

$$\frac{1}{\mathbf{p}^2 + \gamma^2} \rightarrow \frac{2\pi^2}{r} e^{-\gamma r}, \tag{C16b}$$

and some useful identities involving the differential operators are

$$p_i p_j e^{-\gamma r} = -(\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) \left[ \frac{\gamma}{r} + \gamma^2 \right] e^{-\gamma r} - \frac{1}{3} \left[ \gamma^2 - \frac{2\gamma}{r} \right] \delta_{ij} e^{-\gamma r}, \tag{C17a}$$

$$p_i p_j \frac{1}{r} = -\frac{3}{r^3} (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) + \frac{1}{3} 4\pi \delta(\mathbf{r}) \delta_{ij}, \tag{C17b}$$

$$p_i p_j \frac{1}{r} e^{-\gamma r} = \left[ \left[ -\frac{3}{r^3} - \frac{3\gamma}{r^2} - \frac{\gamma^2}{r} \right] (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) + \left[ -\frac{\gamma^2}{r} + 4\pi \delta(\mathbf{r}) \right] \frac{1}{3} \delta_{ij} \right] e^{-\gamma r}, \tag{C17c}$$

$$\frac{1}{\mathbf{p}^2 + \gamma^2} 4\pi \delta(\mathbf{r}) = \frac{1}{r} e^{-\gamma r}, \tag{C17d}$$

$$\frac{1}{\mathbf{p}^2 + \gamma^2} \frac{1}{r} e^{-\gamma r} = \frac{1}{2\gamma} e^{-\gamma r}, \tag{C17e}$$

$$\frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{3}{r^3} (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) \right] e^{-\gamma r} = (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) \left[ -\frac{1}{2r} \right] e^{-\gamma r}, \tag{C17f}$$

$$\frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{3\gamma}{r^2} - \frac{\gamma^2}{r} \right] (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) e^{-\gamma r} = -\frac{\gamma}{2} (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) e^{-\gamma r}, \tag{C17g}$$

where  $\hat{r}_i = r_i / |\mathbf{r}|$  and  $r = |\mathbf{r}|$ . The two  $D$ -wave expressions (C17f) and (C17g) are most easily verified by writing them in the form of differential equations as in Sec. V.

For  $I_2$ , the  $S$ -wave contribution is

$$\begin{aligned} & \frac{\pi^5}{2\gamma^2} (\frac{1}{3} \delta_{ij})^2 \int d^3r e^{-\gamma r} \left[ 4\pi \delta(\mathbf{r}) \frac{1}{\mathbf{p}^2 + \gamma^2} 4\pi \delta(\mathbf{r}) - \left[ -\frac{\gamma^2}{r} + 4\pi \delta(\mathbf{r}) \right] \frac{1}{\mathbf{p}^2 + \gamma^2} 4\pi \delta(\mathbf{r}) \right. \\ & \quad \left. - 4\pi \delta(\mathbf{r}) \frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{\gamma^2}{r} + 4\pi \delta(\mathbf{r}) \right] + \left[ -\frac{\gamma^2}{r} + 4\pi \delta(\mathbf{r}) \right] \frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{\gamma^2}{r} + 4\pi \delta(\mathbf{r}) \right] \right] e^{-\gamma r} \\ & = \frac{\pi^5}{6\gamma} \int d^3r e^{-\gamma r} \left[ \frac{\gamma^2}{r} \frac{1}{\mathbf{p}^2 + \gamma^2} \frac{\gamma^2}{r} \right] e^{-\gamma r} = \frac{\pi^6}{12\gamma}, \tag{C18a} \end{aligned}$$

and the  $D$ -wave contribution is

$$\begin{aligned} & \frac{\pi^5}{2\gamma^2} \int d^3r (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) e^{-\gamma r} \left[ \left[ -\frac{3}{r^3} \right] \frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{3}{r^3} \right] - \left[ -\frac{3}{r^3} \right] \frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{3}{r^3} - \frac{3\gamma}{r^2} - \frac{\gamma^2}{r} \right] \right. \\ & \quad - \left[ -\frac{3}{r^3} - \frac{3\gamma}{r^2} - \frac{\gamma^2}{r} \right] \frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{3}{r^3} \right] \\ & \quad \left. - \left[ -\frac{3}{r^3} - \frac{3\gamma}{r^2} - \frac{\gamma^2}{r} \right] \frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{3}{r^3} - \frac{3\gamma}{r^2} - \frac{\gamma^2}{r} \right] \right] (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) e^{-\gamma r} \\ & = \frac{\pi^5}{2\gamma^2} \int d^3r (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) e^{-\gamma r} \left[ -\frac{3\gamma}{r^2} - \frac{\gamma^2}{r} \right] \frac{1}{\mathbf{p}^2 + \gamma^2} \left[ -\frac{3\gamma}{r^2} - \frac{\gamma^2}{r} \right] (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij}) e^{-\gamma r} = \frac{7\pi^5}{6\gamma^2}. \end{aligned} \tag{C18b}$$

For  $I_3$ , the  $S$ -wave contribution is

$$\frac{\pi^7}{\gamma^2} \int d^3r \left[ \frac{1}{r^2} - \left[ -\frac{\gamma}{2} + \frac{1}{r} \right]^2 \right] (\frac{1}{3} \delta_{ij} e^{-\gamma r})^2 \frac{1}{r} = \frac{7\pi^8}{12\gamma^2}, \tag{C19a}$$

and the  $D$ -wave contribution is

$$\begin{aligned} & \frac{\pi^7}{\gamma^2} \int d^3r \left[ \left[ -\frac{1}{2r} \right]^2 - \left[ \frac{1}{2r} + \frac{\gamma}{2} \right]^2 \right] \\ & \quad \times [e^{-\gamma r} (\hat{r}_i \hat{r}_j - \frac{1}{3} \delta_{ij})]^2 \frac{1}{r} = -\frac{5\pi^8}{6\gamma^2}. \end{aligned} \tag{C19b}$$

The results for the three- and four-loop integrals are listed in Table VIII.

**APPENDIX D: THE MODIFIED DIRAC-COULOMB WAVE FUNCTION**

In Sec. II, we found the three-dimensional equation (2.6a) for the starting wave function

$$(H_e + \mathcal{V})\psi_n = E'_n \psi_n, \tag{D1}$$

where the effective potential is given by

$$\mathcal{V} = V_c \left[ 1 - \beta_e \frac{m_e}{E} \right]. \tag{D2}$$

The total energy  $E$  is defined in (2.1):

$$E = E' + E'', \tag{D3}$$

where  $E'$  and  $E''$  are related through

$$E'^2 - m_e^2 = E''^2 - m_e^2.$$

We need to solve (D1) for the ground state energy  $E'_0$  and wave function  $\psi_0$ . Note that  $\mathcal{V}$  depends on  $E'$  through  $E$ , so that we do not have a linear eigenvalue problem. Our procedure is to find the eigenvalues  $E'_n$  as a function of a parameter  $E$ , which is subsequently adjusted to agree with (D3). Since the dependence of  $E'_n$  on  $E'$  is rather

weak, we could solve for  $E'_n$  iteratively in this manner.

The procedure for solving this equation was developed by Grotch and Yennie (1969); they arrived at a similar equation through a slightly different approximation method. One makes the substitution

$$\psi_n = C \left[ 1 + \beta_e \frac{m_e}{E} \right]^{1/2} \chi_n, \tag{D4}$$

where  $C$  is a normalization constant to be determined later.

After substituting (D4) into (D1), we multiply both sides by

$$\left[ \frac{1 + \beta_e \frac{m_e}{E}}{1 - \frac{m_e^2}{E^2}} \right]^{1/2}.$$

[Note that  $(1 + \beta_e m_e/E)$  is a positive definite matrix, so that its square root is perfectly well defined.] The expression may then be rearranged to give

$$(\alpha_e \cdot \mathbf{p} + \beta_e \bar{m} + \bar{V}_c) \chi_n = \bar{E}'_n \chi_n, \tag{D5}$$

where

$$\bar{V}_c = -\frac{\bar{\alpha}}{r}, \tag{D6a}$$

$$\bar{\alpha} = \alpha(1 - m_e^2/E^2)^{1/2}, \tag{D6b}$$

$$\bar{m} = m_e \frac{1 - E'_n/E}{(1 - m_e^2/E^2)^{1/2}}, \tag{D6c}$$

and

TABLE VI. Results of the integrations for  $K_{14}$  different polynomials.

| $\mathbf{p}^2 \mathbf{p} \cdot \mathbf{p}'$ | $(\mathbf{p} \cdot \mathbf{p}')^2$ | $\mathbf{p}^2 \mathbf{p}'^2$ | $\gamma^2 \mathbf{p} \cdot \mathbf{p}'$ |
|---|------------------------------------|------------------------------|---|
| $2 \ln 2 - \frac{1}{2}$                     | $2 \ln 2 - \frac{1}{2}$            | $2 \ln 2 + \frac{1}{2}$      | 0                                       |

TABLE VII. Results of the integrations for  $K_{15}$  different polynomials.

| $\mathbf{p}^2(\mathbf{p}'^2 - \mathbf{p} \cdot \mathbf{p}')$ | $\mathbf{p} \cdot \mathbf{p}'(\mathbf{p}'^2 - \mathbf{p} \cdot \mathbf{p}')$ | $\mathbf{p}'^2(\mathbf{p}^2 - \mathbf{p} \cdot \mathbf{p}')$ | $\mathbf{p} \cdot \mathbf{p}'(\mathbf{p}^2 - \mathbf{p} \cdot \mathbf{p}')$ |
|--|--|--|---|
| $\frac{1}{2} \ln \frac{m}{2\gamma} - \frac{1}{32}$           | $\frac{1}{4} \ln \frac{m}{\gamma} - \frac{13}{32}$                           | $\frac{1}{4} \ln \frac{m}{2\gamma} + \frac{13}{32}$          | $\frac{5}{32}$  |
|  | $\gamma^2(\mathbf{p}'^2 - \mathbf{p} \cdot \mathbf{p}')$                     | $\gamma^2(\mathbf{p}^2 - \mathbf{p} \cdot \mathbf{p}')$      |   |
|  | $\frac{5}{32}$   | $\frac{3}{32}$   |   |

$$\bar{E}'_n = \frac{E'_n - m_e^2/E}{(1 - m_e^2/E^2)^{1/2}} \tag{D6d}$$

This is just the Dirac equation for a particle of mass  $\bar{m}$  and energy  $\bar{E}'_n$  in a modified Coulomb potential  $\bar{V}_c$ .

The solutions of (D5) in terms of the modified parameters are given by the well-known Coulomb-Dirac wave functions

$$\chi_n^{jm}(\bar{\alpha}\bar{m} \mathbf{r}, \bar{\alpha}), \tag{D7a}$$

while the eigenvalues are given by the usual fine-structure formula

$$\bar{E}'_n = \bar{m}f_n(\bar{\alpha}), \tag{D7b}$$

where the  $f_n$  differ from unity by order  $\bar{\alpha}^2$ :

$$f_n - 1 = O(\bar{\alpha}^2) \tag{D7c}$$

In particular, for the ground state

$$f_0(\bar{\alpha}) = (1 - \bar{\alpha}^2)^{1/2} \approx 1 - \frac{1}{2}\bar{\alpha}^2. \tag{D8a}$$

The eigenvalue  $E'_n$  of our original equation is now expressed in terms of  $\bar{\alpha}$  by combining (D6c) and (D6d) with (D7b). The result is

$$E'_n = m_e \frac{f_n(\bar{\alpha}) + \frac{m_e}{E}}{1 + m_e f_n(\bar{\alpha})/E}. \tag{D8b}$$

Finally, using the property of  $f_n$  given in (D7c), we find

$$E'_n = m_e \left[ 1 + [f_n(\alpha) - 1] \frac{m_\mu^2}{(m_\mu + m_e)^2} + O\left(\alpha^4 \frac{m_e^2}{E^2}\right) \right] \tag{D8c}$$

$$\approx m_e + [f_n(\alpha) - 1] \frac{m_r^2}{m_e}. \tag{D8d}$$

The result for the total energy of the state is then

$$E \approx m_e + m_\mu + [f_n(\alpha) - 1]m_r + O(\alpha^4 m_e^2/m_\mu). \tag{D8e}$$

Thus, to order  $\alpha^2$ , all binding energies are given in terms of the reduced mass. It should also be remarked that the last term of (D8e) does not affect the fine structure, whose corrections are of relative order  $m_e^2/m_\mu^2$ . These re-

sults are perfectly adequate for our treatment of muonium and for the terms which we treat in positronium.

As an illustration, we give the explicit result for the ground-state wave function  $\chi_0(\bar{\alpha}\bar{m} \mathbf{r}, \bar{\alpha})$

$$\chi_0(\bar{\alpha}\bar{m} \mathbf{r}, \bar{\alpha}) = g(r) \begin{pmatrix} \lambda_m \\ i \left[ \frac{1 - f_0(\bar{\alpha})}{1 + f_0(\bar{\alpha})} \right]^{1/2} \frac{\boldsymbol{\sigma}_e \cdot \mathbf{r}}{r} \lambda_m \end{pmatrix}, \tag{D9a}$$

where  $\lambda_m$  is a Pauli spinor and

$$g(r) = \pi^{-1/2} \bar{\gamma}^{3/2} \left[ \frac{1 + f_0(\bar{\alpha})}{\Gamma[2f_0(\bar{\alpha}) + 1]} \right]^{1/2} \times e^{-\bar{\gamma}r(2\bar{\gamma}r)^{f_0(\bar{\alpha})-1}}, \tag{D9b}$$

$$\begin{aligned} \bar{\gamma} &= \bar{m}\bar{\alpha} \\ &\approx m_r \alpha [1 + O(\alpha^2 m_e/m_\mu)]. \end{aligned} \tag{D9c}$$

Recall that

$$\left[ \frac{1 - f_0(\bar{\alpha})}{1 + f_0(\bar{\alpha})} \right]^{1/2} \approx \frac{\bar{\alpha}}{2} + O(\bar{\alpha}^3),$$

so that the coefficient in the lower component of the wave function can be approximated, if desired. In any case, we need the form (D9a) only in evaluating the expectation value of the leading order kernel in Sec. III.C. That calculation reduces to the one carried out by Breit (1930) long ago for the nonrecoil case; the only change is the substitution of modified parameters which take into account "reduced mass" aspects of the recoil, as is apparent in (D9c).

For other kernels, which manifest intrinsic recoil corrections, it is sufficient to approximate (D9) by the usual nonrelativistic form

TABLE VIII. Three and four loop integrals.

| $I_1$                  | $I_2$                    | $I_3$                      |
|------------------------|--------------------------|----------------------------|
| $\frac{\pi^6}{\gamma}$ | $\frac{5\pi^6}{4\gamma}$ | $-\frac{\pi^8}{4\gamma^2}$ |

$$\chi_0 \approx C_{nr} \left[ \begin{array}{c} \lambda_0 e^{-\gamma r} \\ -i\sigma_e \cdot \nabla \\ 2m_r \end{array} \lambda_0 e^{-\gamma r} \right]. \tag{D10}$$

It is noteworthy that the lower component depends on  $m_r$ , rather than  $m_e$ ; however, in the actual wave function  $\psi$ ,  $m_r$  is replaced by  $m_e$  [see (D13)].

The normalization constant is easily determined from

$$1 = C^2 \left\langle \chi \left| 1 + \beta_e \frac{m_e}{E} \right| \chi \right\rangle = C^2 \left[ 1 + f_0(\alpha) \frac{m_e}{E} \right]. \tag{D11}$$

This gives  $C$ . The result may be seen directly from (D9), but it is not special to the ground state. To derive it more generally, use

$$\frac{\partial}{\partial \bar{m}} \langle \chi_n | \alpha_e \cdot \mathbf{p} + \beta_e \bar{m} + \bar{V}_c - \bar{m} f_0(\bar{\alpha}) | \chi_n \rangle = 0, \tag{D12}$$

where the expression is regarded as a function of  $\bar{m}$  and  $\bar{\alpha}$ , treated as independent variables.

Our solution is now

$$\psi_0 = \left[ \frac{1 + \beta_e \frac{m_e}{E}}{1 + f_0(\bar{\alpha}) \frac{m_e}{E}} \right]^{1/2} \chi_0. \tag{D13}$$

**APPENDIX E: CONSTRUCTION OF THE BETHE-SALPETER WAVE FUNCTION**

Although the Bethe-Salpeter wave function plays no direct role in our analysis, it is interesting to see how it can be constructed from our results. It is known [see Lurie *et al.* (1965)] that near poles in  $E$ , the four-point function takes the form

$$G \approx \frac{|n\rangle\langle n|}{E' - \tilde{E}'_n}, \tag{E1}$$

where the numerator is given in terms of the four-dimensional Bethe-Salpeter wave functions  $|n\rangle$ . Hence we have only to find an expression for this residue. Later we will show that the result does satisfy the four-dimensional integral equation of Bethe and Salpeter.

The positions of the bound-state poles of  $G$  are the same as those of  $\hat{G}$ . A little thought shows that for  $E'$  in the vicinity of  $\tilde{E}'_0$ ,  $\hat{G}$  may be written

$$\hat{G} \approx \frac{|\hat{0}; E'\rangle\langle\hat{0}; E'|}{E' - E'_0 - \Sigma(E')}, \tag{E2a}$$

where

$$\begin{aligned} |\hat{0}; E'\rangle &= |\bar{0}\rangle + \sum_{n \neq 0} \frac{|\bar{n}\rangle\langle\bar{n}| N\hat{K} |\bar{0}\rangle}{E' - E'_n} \\ &+ \sum_{n_1 \neq 0} \sum_{n_2 \neq 0} \frac{|\bar{n}_1\rangle\langle\bar{n}_1| N\hat{K} |\bar{n}_2\rangle\langle\bar{n}_2| N\hat{K} |\bar{0}\rangle}{(E' - E'_{n_1})(E' - E'_{n_2})} \\ &+ \dots, \end{aligned} \tag{E2b}$$

with a similar expression for  $\langle\hat{0}; E'|$ . Recall that the states  $|\bar{n}\rangle$  and the eigenvalues  $E'_n$  depend on  $E'$ . The pole in (E2a) occurs at  $E' = \tilde{E}'_0$ ; and according to (2.11a), the Bethe-Salpeter wave function is then given by

$$|0\rangle = (1 + \Gamma_l) |\hat{0}; \tilde{E}'_0\rangle, \tag{E3}$$

where  $E'$  in  $\Gamma_l$  is also fixed at  $\tilde{E}'_0$ . We are not attempting to determine the normalization of the wave function, but only its structure.

The structure of  $\Gamma_l$  is arrived at by recalling the steps leading from (2.10a) to (2.11a). After iterating  $G$  using (2.8) until a factor of  $Q_c$  is obtained, we find in (2.10a) a term with the structure

$$\begin{aligned} (RQ_c + SQSQ_c + SQSQSQ_c + \dots)G \\ = \left[ RQ_c + \frac{1}{1 - SQ} SQSQ_c \right] G. \end{aligned} \tag{E4a}$$

The iteration of this term produces  $\Gamma_l$ , which then satisfies the integral equation

$$\Gamma_l = \left[ RQ_c + \frac{1}{1 - SQ} SQSQ_c \right] (1 + \Gamma_l) \tag{E4b}$$

or

$$\Gamma_l = SQ\Gamma_l + (RQ_c + SQN\bar{S}Q_c)(1 + \Gamma_l). \tag{E4c}$$

Incidentally,  $\hat{K}$  is easily expressed in terms of  $\Gamma_l$ :

$$\hat{K} = \delta Q_c + Q_c \Gamma_l. \tag{E4d}$$

We can also derive an integral equation for  $|\hat{0}\rangle$ . From (2.11b) we see that

$$\hat{G} = \bar{G} + \bar{G}N\hat{K}\hat{G}. \tag{E5}$$

Taking the residue of the pole at  $E' = \tilde{E}'_0$  on both sides of (E5), we find (using the fact that  $\bar{G}$  has no pole there) that

$$|\hat{0}\rangle = \bar{G}N\hat{K}|\hat{0}\rangle, \tag{E6}$$

which is compatible with (E2b). Acting on this with  $\bar{S}\mathcal{Y}$  and using (2.9b), we find, after a little rearrangement, that

$$\begin{aligned} \bar{S}\mathcal{Y}|\hat{0}\rangle &= (\bar{G} - \bar{S})N\hat{K}|\hat{0}\rangle \\ &= |\hat{0}\rangle - \bar{S}N\hat{K}|\hat{0}\rangle \end{aligned}$$

or, using (E4d), we find that

$$|\hat{0}\rangle = \bar{S}NQ_c(1 + \Gamma_l)|\hat{0}\rangle. \tag{E7}$$

The relation that we wish to prove is the integral equation for the Bethe-Salpeter wave function:

$$|0\rangle = S(Q_c + Q)|0\rangle. \quad (\text{E8})$$

To show this, we rearrange the right-hand side of (E3) using (E4c) and (E7). This gives

$$|0\rangle = (\bar{S}N + R)Q_c(1 + \Gamma_l)|\hat{0}\rangle + SQ[\Gamma_l + N\bar{S}Q_c(1 + \Gamma_l)]|\hat{0}\rangle.$$

Using (2.9a) and (E7) once again, we find that this reduces to (E8).

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