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TWO-BODY BOUND STATES IN QUANTUM ELECTRODYNAMICS*

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Abstract

We examine novel formulations of the two-body bound state problem in quantum field theory. While equal in rigor, these have several calculational advantages over the traditional Bethe-Salpeter formalism. In particular there exist exact solutions of the bound state equations for a Coulomb-like interaction in quantum electrodynamics. The corrections to such zeroth-order solutions can be systematically computed in a simple perturbation theory. We illustrate these methods by computing corrections to the orthopositronium decay rate and to the ground state splittings in positronium and muonium.

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Preface and Acknowledgements

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Much of the work described here has already been published elsewhere. Most of Section III appears in References 8, 10 and 11. Section IV elaborates ideas first presented in the Appendix of Reference 9.

Finally, I must thank my wife Deborah who read the original manuscript and corrected my sometimes rather unconventional (to put it kindly) sentence structure and punctuation. I, not she, am responsible for what remains uncorrected.

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1. INTRODUCTION

In recent years, the ground state hyperfine splittings in positronium (e^+e^-) and muonium (μ^+e^-) have been measured with great precision (1 ppm or better).^{1,2,3} Measurements such as these allow a detailed test of our understanding of two-body bound states in quantum field theory and particularly in quantum electrodynamics (QED). Any analysis of these atoms must account fully for the relativistic dynamics and interactions of both constituents. Furthermore, unlike the situation for hydrogen, strong interactions have almost no measurable effect on the spectra of these pure QED systems.

In the past, most calculations have employed the covariant Bethe-Salpeter (BS) formalism.⁴ High order calculations within this framework have been greatly handicapped by the lack of a tractable, systematic computational procedure, and in fact, theory has lagged far behind experiment in precision. It is essential that an exactly soluble zeroth-order problem, incorporating the basic physics, exists when computing corrections to energy levels or decay rates in high orders of perturbation theory. Unfortunately, analytic solutions of the BS equation have not been found for any approximation of the QED (fermion) interaction.⁵ Formerly, the BS wave function has been approximated by iterating the equation. While useful when computing first order corrections, this procedure fails completely for higher order calculations.

Much of the difficulty in solving the BS equation arises because of its dependence upon such superfluous variables as the relative time or energy of the constituents. These can be removed when the interaction is instantaneous, resulting in the Salpeter equation.⁶ Still neither the

Salpeter equation nor the related Breit equation is readily solved for a Coulomb interaction and the central problem remains.

A major advance is to realize that the form of the bound state equation can be greatly altered, with no loss of rigor, by a suitable redefinition of the interaction kernel or "quasi-potential."⁷ From this viewpoint, the BS equation is but one of an infinity of equivalent bound state equations. This new freedom in designing formalisms can be exploited to incorporate more physics in simpler equations. Furthermore, the basic equations can be tailored to the particular system of interest.

In this report we apply these ideas to the atomic physics of QED atoms. We will describe two new relativistic two-body formalisms--the first being most useful when binding is weak (e.g., positronium, muonium),⁸ the second when constituents differ greatly in mass (e.g., muonium, high Z atoms).⁹ Both are equal in rigor to the BS formalism but have clear calculational advantages. Outstanding among these is the existence in each case of Coulomb-like kernels for which the exact analytic solutions of the bound state equations are known. Corrections to these zeroth-order solutions can then be systematically elaborated in a simple perturbation series. To illustrate the procedure, we compute the $O(\alpha)$ and leading $O(\alpha^2)$ corrections to the decay rate of orthopositronium.^{10,11} We also compute the leading $O(\alpha^2)$ corrections to the hyperfine splitting in muonium and positronium.^{8,9} Most of these results were computed for the first time using the methods described below.

In Section II, we review the general features of a bound state formalism. We also describe the BS equation and its shortcomings as a calculational tool. In Section III, we introduce a new bound state equation which reduces to a Schrodinger equation for a single effective particle.

This formalism is applied in a calculation of corrections to the decay rate of orthopositronium. Finally, in Section IV, we describe a formalism, pioneered by F. Gross, which reduces to an effective Dirac equation. This is applied in computing the $O(\alpha^2 \ln \alpha^{-1})$ corrections to the hyperfine structure.

II. ANATOMY OF A BOUND STATE FORMALISM

A. The General Treatment

Most analyses of two-body bound states in field theory focus upon the analytic structure of the (truncated) two-particle Green's function G_T as a function of the total energy. Unitarity requires that G_T have poles at the bound state energies (P^0), and that these poles have factorized residues. That is

$$G_T(kqP) \rightarrow \frac{\phi(kP) \bar{\phi}(qP)}{P^0 - P_n^0} \quad \text{as } P^0 \rightarrow P_n^0 \quad (11.1)$$

where P is the total four-momentum, and k and q are the relative momenta of the constituents. The goal in applying any bound state formalism is to locate these poles and to determine the corresponding wave functions ϕ .

In field theory, G_T is specified by a perturbative expansion in the coupling constant. However, the bound state poles of G_T are also poles in G_T considered as a function of the coupling constant (with P held fixed), and as such cannot appear in any finite order of perturbation theory. We must go beyond perturbation theory if we are to analyse the bound states of a field theory. We accomplish this by iterating some basic interaction in a Lippman-Schwinger or Dyson equation having the general form:

$$G_T(P) = K(P) + K(P) S(P) G_T(P) \quad (11.2)$$

where integrations over relative four-momenta are implicit. Here $K(P)$ is the interaction kernel and $S(P)$ is a two-particle propagator. The propagator $S(P)$ is arbitrary and, once selected, determines the interaction $K(P)$ as well as the final form of the bound state equations. The expansion in the coupling constant of $K(P)$ follows from Eq. (11.2) and the

expansion for $G_T(P)$:

$$K(P) = G_T(P) \frac{1}{1 + S(P) G_T(P)}$$

$$= G_T(P) - G_T(P) S(P) G_T(P) + \dots \quad (II.3)$$

If $S(P)$ is well chosen, the lowest order terms in $K(P)$ contain the basic physics; the remaining terms can then be treated perturbatively. The optimal choice is dictated 1) by the qualitative features of the system under study, and 2) by the need for a bound state equation which is exactly solvable for some approximate kernel.

It is convenient to introduce a two-particle Green's function having external fermion propagators:

$$G(P) = S(P) + S(P) G_T(P) S(P)$$

$$= S(P) + S(P) K(P) G(P) \quad (II.4)$$

Clearly $G(P)$, like $G_T(P)$, has poles at the bound state energies P_n^0 :

$$G(P) \rightarrow \frac{\psi_n \bar{\psi}_n}{P^0 - P_n^0} \text{ as } P^0 \rightarrow P_n^0 \quad (II.5)$$

Substituting this in Eq. (II.4) and equating the residues of the pole on each side leads immediately to the bound state equation

$$S^{-1}(P_n) \psi_n = K(P_n) \psi_n \quad (II.6)$$

--an eigenvalue equation for the energies of the bound states and their wave functions.

Equations (II.4) and (II.5) fix the normalization of the wave functions.

To see this we rewrite (II.4) as

$$G(P) S^{-1}(P) = 1 + G(P) K(P)$$

Multiplying this equation on the right by ψ_n and Eq. (II.6) on the left by $G(P)$, and then subtracting the two, we obtain:

$$G(P) W(P, P_n) \psi_n = \frac{\psi_n}{P^0 - P_n^0} \quad (II.7)$$

where

$$W(P, P_n) = \frac{S^{-1}(P) - S^{-1}(P_n)}{P^0 - P_n^0} - \frac{K(P) - K(P_n)}{P^0 - P_n^0}$$

$$= \frac{\partial}{\partial P^0} [S^{-1}(P) - K(P)]_{P^0 = P_n^0} \text{ as } P^0 \rightarrow P_n^0$$

Evaluating Eq. (II.7) at the bound state pole we obtain the condition required for orthonormality

$$\bar{\psi}_m W(P_m, P_n) \psi_n = \delta_{mn} \quad (II.8)$$

B. Perturbation Theory for Bound States

In practice, we solve Eq. (II.6) only (or some approximate kernel, $K_0(P)$). The stationary perturbation theory usually applied to the Schrödinger equation is easily adapted to this problem, and may be used to correct energies and wave functions.¹² For simplicity we work in the rest frame $P = (E, 0, 0, 0)$ and restrict our attention to non-degenerate levels. Let $\{\psi_n^0\}$ be the eigenfunctions with total energies $\{E_n^0\}$ of Eq. (II.6) with kernel $K_0(E)$, and let $G_0(E)$ be the corresponding Green's function. If

$G(E)$ is the Green's function for kernel $K(E) = K_0(E) + \delta K(E)$, then

$$G(E) = G_0(E) + G_0(E) \delta K(E) G(E) \\ = \sum_{j=0}^{\infty} (G_0(E) \delta K(E))^j G_0(E) \quad (11.9)$$

and $G(E)$ has poles at the perturbed energy levels $\{E_n\}$:

$$G(E) \rightarrow \frac{\bar{\psi}_n \psi_n}{E - E_n} \quad \text{as } E \rightarrow E_n$$

We define a closed integration contour C_n in E -space encircling E_n , E_n^0 and no other poles of G , G_0 or K . Cauchy's theorem implies

$$E_n [\bar{\psi}_n^0 W(E_n^0 E_n) \psi_n] [\psi_n W(E_n E_n^0) \psi_n^0] \\ = \oint_{C_n} \frac{E dE}{2\pi i} \bar{\psi}_n^0 W(E_n^0 E) G(E) W(E E_n^0) \psi_n^0 \\ [\bar{\psi}_n^0 W(E_n^0 E_n) \psi_n] [\bar{\psi}_n W(E_n E_n^0) \psi_n^0] \\ = \oint_{C_n} \frac{dE}{2\pi i} \bar{\psi}_n^0 W(E_n^0 E) G(E) W(E E_n^0) \psi_n^0$$

The integrations can be expressed in terms of known quantities through use of Eq. (11.9) to remove $G(E)$ in favor of $\delta K(E)$ and $G_0(E)$. The result is an expansion for E_n in powers of δK (using Eq. (11.7)):

$$E_n = E_n^0 + \frac{\oint_{C_n} \frac{dE}{2\pi i} \frac{1}{E - E_n^0} \bar{\psi}_n^0 \delta K(E) \sum_{j=0}^{\infty} [G_0(E) \delta K(E)]^j \psi_n^0}{1 + \oint_{C_n} \frac{dE}{2\pi i} \frac{1}{(E - E_n^0)^2} \bar{\psi}_n^0 \delta K(E) \sum_{j=0}^{\infty} [G_0(E) \delta K(E)]^j \psi_n^0}$$

The contour integrations in each term of the expansion can be readily performed as the only poles implicit in the integrand occur in $G_0(E)$ at E_n^0 and the residue is known (Eq. (11.5)). We obtain finally the familiar perturbation series:

$$E_n = E_n^0 + \left(\bar{\psi}_n^0 \delta K \psi_n^0 \right) \left[1 + \bar{\psi}_n^0 \frac{\partial}{\partial E} \delta K \psi_n^0 \right]_{E=E_n^0} \\ + \left[\bar{\psi}_n^0 \delta K \left(G_0 - \frac{\bar{\psi}_n^0 \psi_n^0}{E - E_n^0} \right) \delta K \psi_n^0 \right]_{E=E_n^0} + O(\delta K^3) \quad (11.10)$$

Similar arguments give the perturbed wave functions:

$$\psi_n \approx \psi_n^0 + \oint_{C_n} \frac{dE}{2\pi i} \sum_{j=1}^{\infty} [G_0(E) \delta K(E)]^j \frac{\psi_n^0}{E - E_n^0} \\ = \psi_n^0 \left[1 + \bar{\psi}_n^0 \frac{\partial}{\partial E} \delta K \psi_n^0 \right]_{E=E_n^0} \\ + \left(G_0 - \frac{\bar{\psi}_n^0 \psi_n^0}{E - E_n^0} \right) \delta K \psi_n^0 \Big|_{E=E_n^0} + O(\delta K^2)$$

The perturbed wave functions are useful primarily in computing scattering amplitudes. They will not be needed in what follows.

Decay channels shift the bound state poles of G below the real axis. The decay width of the n^{th} level is simply

$$\Gamma_n = -2 \mathcal{I}m E_n \quad (11.11)$$

and may be calculated perturbatively from Eq. (11.10).¹³

C. An Example: The Bethe-Salpeter Equation

Equation (II.4) becomes the BS equation⁴ if we choose the propagator

$$S(kP) = \frac{i}{\tau_1 \not{P} + \not{k} - m_1} \frac{i}{\tau_2 \not{P} - \not{k} - m_2} \quad i = \frac{m_1}{m_1 + m_2}$$

The bound state equation is Eq. (II.6)

$$(\tau_1 \not{P} + \not{k} - m_1)(\tau_2 \not{P} - \not{k} - m_2) \psi_{BS}(kP) = - \int \frac{d^4 q}{(2\pi)^4} K_{BS}(kqP) \psi_{BS}(qP)$$

The kernel K_{BS} is the sum of all two-particle irreducible diagrams (Eq. (II.3), Fig. 1). This kernel is dominated by the static single-photon interaction in nonrelativistic QED atoms. When the kernel is static (i.e., independent of relative energy), the BS equation is greatly simplified by integrating over the relative energy. This results in a three-dimensional formalism whose propagator in the atom's rest frame is

$$S(kP) = 2\pi i \delta(k^0) \left[\frac{\Lambda_+^{(1)}(\vec{k}) \Lambda_+^{(2)}(-\vec{k})}{P^0 - E_1(k) - E_2(k)} - \frac{\Lambda_-^{(1)}(\vec{k}) \Lambda_-^{(2)}(-\vec{k})}{P^0 + E_1(k) + E_2(k)} \right] \gamma_o^{(1)} \gamma_o^{(2)}$$

$$= \frac{2\pi i \delta(k^0)}{P^0 - H_1(\vec{k}) - H_2(-\vec{k})} \left[\Lambda_+^{(1)} \Lambda_+^{(2)} - \Lambda_-^{(1)} \Lambda_-^{(2)} \right] \gamma_o^{(1)} \gamma_o^{(2)} \quad (\text{II.12})$$

where

$$E_i(k) = \sqrt{k^2 + m_i^2} \quad \Lambda_{\pm}(\vec{k}) = \frac{E(k) \pm (\vec{\alpha} \cdot \vec{k} + \beta m)}{2E(k)}$$

$$H(\vec{k}) = \vec{\alpha} \cdot \vec{k} + \beta m = E(k)(2\Lambda_+(\vec{k}) - 1)$$

Fig. 1. The two-particle irreducible BS kernel.

The resulting bound state equation is the 'Salpeter equation':⁶

$$[P^0 - H_1(\vec{k}) - H_2(-\vec{k})] \psi(\vec{k}) = [\Lambda_+^{(1)} \Lambda_+^{(2)} - \Lambda_-^{(1)} \Lambda_-^{(2)}] \gamma_0^{(1)} \gamma_0^{(2)} \\ \times \int \frac{d^3 q}{(2\pi)^3} \frac{1}{K(\vec{k}, \vec{q}, P)} \psi(\vec{q}) \quad (II.13)$$

It can be made exact by incorporating retardation corrections into the kernel via Eq. (II.3). Still this equation allows no simple solutions for QED atoms. It also illustrates a basic defect in the BS formalism. In the Coulomb-ladder approximation ($K = -e^2 \gamma_0^{(1)} \gamma_0^{(2)} / |\vec{k} - \vec{q}|^2$), Eq. (II.13) becomes

$$(m_1 + \epsilon - \vec{\alpha} \cdot \vec{k} - \beta m_1) \psi(\vec{k}) = \Lambda_+^{(1)}(k) \int \frac{d^3 q}{(2\pi)^3} \frac{-e^2}{|\vec{k} - \vec{q}|^2} \psi(\vec{q})$$

when $m_2 \rightarrow \infty$ and where ϵ is the binding energy. This is not the Dirac equation, which is the correct limit, because of the $\Lambda_+^{(1)}(k)$ on the left hand side. The antiparticle component of the Dirac propagator is completely suppressed. The Dirac equation is recovered only when all cross-ladder diagrams of all orders are included in K . The failure of the BS Ladder approximation in the infinite mass limit is not serious for nonrelativistic atoms, but demonstrates that the formalism is remarkably inefficient in analysing the relativistic problem.

Breit suggested that the projection operators in Eq. (II.13) be omitted.¹⁴ The equation then has the correct infinite mass limit but is still quite difficult to solve.

We mention one final problem with the BS formalism--the lack of gauge invariance. The wave functions, kernels and Green's functions are not

gauge invariant, though physically measurable quantities such as spectra and decay rates must be. The Coulomb gauge seems to be optimal for atomic physics insofar as it incorporates the most physics in the simplest graphs. The Feynman gauge used in the ladder approximation, for example, results in spurious terms in the binding energy of $O(\alpha^3 \ln \alpha)$ and $O(\alpha^3)$.¹⁵ These terms, which persist even in the infinite mass limit, are cancelled by an infinite number of cross-ladder diagrams. They arise because the Coulomb propagator has mass-shell singularities in this gauge. These unphysical Coulomb photons, which never appear in physical gauges such as the Coulomb gauge, are introduced to make the theory explicitly covariant. However, they must and do ultimately decouple.

The major defect in the BS approach has been the lack of a soluble zeroth order problem approximating the QED atom. Even given a solution, the formalism is awkward since the wave functions depend not only upon the relative position (or momentum) of the constituents but on the relative time (or energy) as well. These problems are overcome in the new treatments discussed in what follows. In addition, the other problems touched upon above (i.e., gauge invariance, the infinite mass limit) are remedied with varying degrees of success.

A. Introduction

1. We determine exact solutions of the bound state equations for a simple Coulomb-like interaction. The wave functions are essentially just the usual Schrodinger wave functions for the hydrogen atom.
2. The corrections to this zeroth-order problem can be elaborated in a systematic perturbation series.
3. The unperturbed two-particle Green's function can be expressed in a number of simple analytic forms. This is important when computing in second order perturbation theory (Eq. (II.10)).
4. As the exact unperturbed wave functions are finite at the origin, the expectation value of the one-photon annihilation kernel (in positronium) is finite. This is not the case in the usual RS approach where this quantity can be made finite only after an infinite order (in α) renormalization of the annihilation vertices. In the formalism described below, all infinities related to renormalization can be removed order by order in precisely the way on-shell amplitudes are treated. This feature greatly simplifies the analysis and numerical evaluation of higher order terms.

- The Dirac fine structure is not included in the unperturbed QED solutions. The fine structure of atoms with constituents of equal mass differs considerably in character from that of atoms with a large mass ratio. It is quite difficult to create a formalism which naturally accommodates both cases and still admits analytic solutions comparable in simplicity to those presented below. The fine structure terms omitted here are of $O((Z\alpha)^4)$ and are easily handled in perturbation theory when the atoms are nonrelativistic ($Z\alpha \ll 1$). Thus, although the formalism is completely general, it is most conveniently applied when the binding energies are small.

As discussed in Section II.C, the static single-photon interaction dominates in weakly bound QED atoms. Furthermore, the $A A_0$ term of the two-fermion BS propagator in this case (Eq. (II.124)) contributes only to $O((Z\alpha)^5)$. This suggests that we construct a formalism with propagator

$$S(kP) = 2\pi i^k \left(k^{(0)} + \dots + (-k)^{(k-1)} \right) \begin{pmatrix} 1 \\ 0 \end{pmatrix}_0 \begin{pmatrix} 2 \\ 0 \end{pmatrix}_0 \quad (111.1)$$

The corresponding two-particle Green's function satisfies an equation

$$\begin{aligned} \bar{G}(\vec{k} \vec{q} P) &= \frac{\Lambda_+^{(1)}(\vec{k}) \Lambda_+^{(2)}(-\vec{k})}{p^0 - E_1(k) - E_2(k)} \gamma_o^{(1)} \gamma_o^{(2)} \left\{ (2\pi)^3 \delta^3(\vec{k} - \vec{q}) + \int \frac{d^3 r}{(2\pi)^3} i \bar{K}(\vec{k} \vec{r} P) \bar{G}(\vec{r} \vec{q} P) \right\} \\ &= \frac{\Lambda_+^{(1)} \Lambda_+^{(2)}}{p^0 - E_1 - E_2} \left\{ (2\pi)^3 \delta^3(k - q) + G_T \frac{\Lambda_+^{(1)} \Lambda_+^{(2)}}{p^0 - E_1 - E_2} \gamma_o^{(1)} \gamma_o^{(2)} \right\} \quad (III.2) \end{aligned}$$

where $\bar{G}_T$ is related to the complete four-point function (Eq. (II.2)) by

$$\bar{G}_T(k q P) = \lim_{k^0, q^0 \rightarrow 0} i G_T(k q P)$$

Equation (III.2) is exact only if $\bar{K}$ is defined as in Eq. (II.3). In terms of the two-particle irreducible BS kernel K_{BS} , we have (Fig. 2a):

$$\begin{aligned} \bar{K}(\vec{k} \vec{q} P) &= K_{BS}(k q P) \Big|_{k^0=q^0=0} + \int \frac{d^4 r}{(2\pi)^4} K_{BS}(k r P) \left\{ \frac{i}{i_1 p + \not{r} - m_1} ; \frac{i}{i_2 p - \not{r} - m_2} \right. \\ &\quad \left. - 2\pi i \delta(r^0) \frac{\Lambda_+^{(1)} \Lambda_+^{(2)}}{p^0 - E_1 - E_2} \right\} K_{BS}(r q P) \Big|_{k^0=q^0=0} + \dots \quad (III.3) \end{aligned}$$

In this fashion, effects due to retardation and the Λ_+ terms are reintroduced into the kernel. As mentioned earlier, the first term in Eq. (III.3) dominates when the binding is weak, and the remaining terms may then be incorporated perturbatively.

Equation (III.2) is far simpler than the BS equation because we have chosen to consider $G_T(k q P)$ only at $k^0 = q^0 = 0$.¹⁷ The location of bound state poles is unaffected by the relative energy of the constituents,¹⁸ and so

$$\boxed{\bar{K}} = \boxed{K} + \left[\boxed{K} \boxed{K} - \boxed{K} \boxed{K} \right] + \dots \quad (a)$$

$$\begin{array}{c} \tau_2 P-k \\ \nearrow \\ \psi \\ \nwarrow \\ \tau_1 P+k \end{array} = \begin{array}{c} \tau_2 P-q \\ \nearrow \\ \psi \\ \nwarrow \\ \tau_1 P+q \end{array} \boxed{\bar{K}} \begin{array}{c} \nearrow \\ \tau_2 P-k \\ \nwarrow \\ \tau_1 P+q \end{array} \quad (b)$$

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Fig. 2a. Definition of the effective kernel in terms of the BS kernel (Fig. 1).

Fig. 2b. The bound state equation.

there is no need to retain this excess degree of freedom when computing energy levels or decay rates. Furthermore, when the BS kernel is static, G_T is independent of k^0 and q^0 , and solving Eq. (III.2) is then equivalent to solving the BS equation.¹⁹

From Eq. (II.6) we find that the bound state equation here is (Fig. 2b)

$$(P^0 - E_1(k) - E_2(k)) \psi(\vec{k}) = \Lambda_+^{(1)}(\vec{k}) \Lambda_+^{(2)}(-\vec{k}) \gamma_0^{(1)} \gamma_0^{(2)} \int \frac{d^3 q}{(2\pi)^3} i \vec{k} \cdot (\vec{k} + \vec{q}) \psi(\vec{q})$$

$$\Lambda_-^{(1)}(\vec{k}) \psi(\vec{k}) = \Lambda_-^{(2)}(-\vec{k}) \psi(\vec{k}) = 0 \quad (\text{III.4})$$

This wave function has 16 spinor components.

Notice that the spinor structure of $\psi(\vec{k})$ follows immediately from Eq. (III.4):

$$\psi(\vec{k}) = \sum_{\lambda\lambda'} \frac{u^{(1)}(\vec{k}\lambda) u^{(2)}(-\vec{k}\lambda')}{\sqrt{4E_1(k)E_2(k)}} \phi(\vec{k})_{\lambda\lambda'} \quad (\text{III.5})$$

where $u(\vec{k}\lambda)$ is the usual free particle Dirac spinor ($\bar{u}u = 2m$), and ϕ has four components. Defining

$$\tilde{G}(\vec{k}\vec{q}P)_{\lambda'\mu'\lambda\mu} = \frac{u^{(1)}(\vec{k}\lambda') u^{(2)}(-\vec{k}\mu')}{\sqrt{4E_1(k)E_2(k)}} \bar{G}(\vec{k}\vec{q}P) \gamma_0^{(1)} \gamma_0^{(2)} \frac{u^{(1)}(\vec{q}\lambda) u^{(2)}(-\vec{q}\mu)}{\sqrt{4E_1(q)E_2(q)}}$$

$$\tilde{\chi}(\vec{k}\vec{q}P)_{\lambda'\mu'\lambda\mu} = \frac{\bar{u}^{(1)}(\vec{k}\lambda') \bar{u}^{(2)}(-\vec{k}\mu')}{\sqrt{4E_1(k)E_2(k)}} \bar{K}(\vec{k}\vec{q}P) \frac{u^{(1)}(\vec{q}\lambda) u^{(2)}(-\vec{q}\mu)}{\sqrt{4E_1(q)E_2(q)}}$$

we can rewrite Eqs. (III.2) and (III.4):

$$\tilde{G}(\vec{k}\vec{q}P) = \frac{1}{P^0 - E_1(k) - E_2(k)} \left\{ (2\pi)^3 \delta^3(\vec{k} - \vec{q}) + \int \frac{d^3 r}{(2\pi)^3} i \vec{k} \cdot (\vec{k} + \vec{r}) G(\vec{r}\vec{q}P) \right\}$$

$$+ \frac{\tilde{\chi}(\vec{k}\vec{q}P) \phi^*(\vec{q})}{P^0 - P_n^0} \quad \text{as } P^0 \rightarrow P_n^0 \quad (\text{III.6a})$$

$$(P^0 - E_1(k) - E_2(k)) \phi(\vec{k}) = \int \frac{d^3 q}{(2\pi)^3} i \vec{k} \cdot (\vec{k} + \vec{q}) \phi(\vec{q}) \quad (\text{III.6b})$$

Wave functions ϕ and ϕ^* satisfy the orthonormality relation Eq. (II.8)

with weight:

$$W(\vec{k}\vec{q}P_m P_n) = (2\pi)^3 \delta^3(\vec{k} - \vec{q}) - \frac{i \vec{k} \cdot (\vec{k} + \vec{q}) P_m - i \vec{k} \cdot (\vec{k} + \vec{q}) P_n}{P_m^0 - P_n^0} \quad (\text{III.7})$$

Perturbation theory (Section II.C) can be expressed in terms of ϕ , ϕ^* , $\tilde{K}$ and $\tilde{G}$ or in terms of ψ , $\bar{\psi}$, $\tilde{K}$ and $\tilde{G}$.

B. The Unperturbed Problem in QED

Equation (III.6b) is rendered more tractable by multiplying both sides by $N(k)^2/N(k)$ where²⁰

$$N(k) = \left(\frac{(P_0^2 + E_1(k) + E_2(k))(P_0^2 - (E_1(k) - E_2(k))^2)}{2P_0(P_0^2 - (m_1 - m_2)^2)} \right)^{1/2}$$

$$= 1 + \frac{k^2}{8m_1^2} - \frac{1}{8} \frac{k^2}{m_1 m_2} - \frac{1}{4(m_1 + m_2)^2} + \dots \quad |\vec{k}| \ll m$$

$$P^0 = P^0 - m_1 - m_2$$

and

$$m = \frac{m_1 m_2}{m_1 + m_2}$$

is the reduced mass. Note that $N(k) \sim 1$ when k is nonrelativistic, and therefore, low energy behavior is little changed by this factor. The resulting equation is

$$\left(\epsilon - \frac{k^2}{2m} \right) \frac{\phi(\vec{k})}{N(k)} = \int \frac{d^3 q}{(2\pi)^3} N(k) N(q) iK(\vec{k} \vec{q} \vec{p}) \frac{\phi(\vec{q})}{N(q)}$$

This is just a Schrodinger equation for an effective particle with "binding energy" and "mass"

$$\epsilon = \frac{p_o^2 - (m_1 + m_2)^2}{2p_o} = \epsilon - \frac{e^2}{2(m_1 + m_2)} + \dots$$

$$\epsilon = \frac{p_o^2 - (m_1 + m_2)^2}{4p_o} = m + e \left(\frac{1}{2} - \frac{m}{m_1 + m_2} \right) + \dots$$

We emphasize that this equation is exact and equivalent to Eqs. (III.4) and (III.6b).

For QED bound states, the choice of zeroth-order kernel is now obvious:

$$iK_o(\vec{k} \vec{q} \vec{p}) = \frac{-e^2}{|\vec{k} - \vec{q}|^2} \frac{1}{N(k) N(q)}$$

as then Eq. (III.6b) reduces to the nonrelativistic Coulomb equation

$$\left(\epsilon - \frac{k^2}{2m} \right) \frac{\phi(\vec{k})}{N(k)} = \int \frac{d^3 q}{(2\pi)^3} \frac{e^2}{|\vec{k} - \vec{q}|^2} \frac{\phi(\vec{q})}{N(q)}$$

The eigenfunctions are simply related to the nonrelativistic hydrogen wave functions with m replaced by m :

$$\phi(\vec{k}) = \frac{N(k)}{\sqrt{1 + \frac{k^2}{m^2}}} i_{\text{Sch}}(\vec{k}; m) \quad n = 1, 2, \dots$$

$$\chi_n(\vec{k}) = \frac{\beta_n^{(1)}(\vec{k}) \beta_n^{(2)}(-\vec{k})}{\sqrt{4 E_1(k) E_2(k)}} \phi(\vec{k})$$

The normalization is fixed by Eqs. (II.8) and (III.7). Note that $\phi(x=0) = \int d^3 k \chi(\vec{k})$ is always finite in the unperturbed problem. The unperturbed energy levels follow by solving

$$\chi(P^0) = -\frac{e^2}{2m^2} \chi(P^0)$$

$$\chi(P^0) = (m_1 + m_2) \left(1 - \frac{e^2}{m^2} \frac{m}{m_1 + m_2} \right)$$

$$m_1 + m_2 = -\frac{e^2}{2m^2} + \frac{e^2}{8m^2} \left(1 - \frac{m}{m_1 + m_2} \right) + O(e^4)$$

It is readily demonstrated that the remaining $O(e^4)$ terms are due to

the following static kernels (in Coulomb gauge):

a) Relativistic corrections to single Coulomb exchange (Fig. 3a):

$$\begin{aligned}
 i\delta \bar{K}_C &= \frac{-e^2}{|\vec{k}-\vec{q}|^2} \gamma_0^{(1)} \gamma_0^{(2)} = i\bar{K}_0 \\
 \Rightarrow i\delta \hat{K}_C &= \frac{-e^2}{|\vec{k}-\vec{q}|^2} \left\{ \frac{\vec{k} \cdot \vec{q}}{4m^2} - \frac{\vec{k}^2 + \vec{q}^2 + 4\vec{k} \cdot \vec{q}}{8m_1 m_2} - \frac{\epsilon}{2(m_1 + m_2)} \right. \\
 &\quad \left. + \frac{i\vec{k} \times \vec{q} \cdot \vec{\sigma}_1}{4m_1^2} + \frac{i\vec{k} \times \vec{q} \cdot \vec{\sigma}_2}{4m_2^2} \right\} \quad (111.8)
 \end{aligned}$$

b) Single transverse photon exchange (Fig. 3b):

$$\begin{aligned}
 i\delta \bar{K}_T &= \frac{e^2}{|\vec{k}-\vec{q}|^2} \gamma_1^{(1)} \gamma_1^{(2)} \delta_{\perp}^{ij} (k-q) \\
 \Rightarrow i\delta \hat{K}_T &= \frac{e^2}{|\vec{k}-\vec{q}|^2} \left\{ \frac{(\vec{k} \cdot \vec{q})^2 - \vec{k}^2 \vec{q}^2}{m_1 m_2 |\vec{k}-\vec{q}|^2} - \frac{i\vec{k} \times \vec{q} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2)}{2m_1 m_2} \right. \\
 &\quad \left. + \frac{(\vec{k}-\vec{q}) \times \vec{\sigma}_1 \cdot (\vec{k}-\vec{q}) \cdot \vec{\sigma}_2}{4m_1 m_2} \right\} \quad (111.8b)
 \end{aligned}$$

c) Single photon annihilation (positronium only, Fig. 3c):

$$\begin{aligned}
 i\delta \bar{K}_A &= \frac{\gamma_5 \cdot \gamma_1}{p_0^2} e^2 \\
 \Rightarrow i\delta \hat{K}_A &= \frac{e^2}{8m_1 m_2} (3 + \vec{\sigma}_1 \cdot \vec{\sigma}_2) \quad m_1 = m_2 \quad (111.8c)
 \end{aligned}$$

(a)

(b)

(c)

••• Coulomb interaction
 --- Transverse Photon
 ~~~~~ K_0 ~~~~~

Fig. 3. Kernels contributing to $\psi\psi^*\psi\psi^*$ in binding energies.

Only the dominant parts of each kernel have been exhibited.

These kernels are important for the analysis presented in Section III.D.

We will also require the ground state ($n = 1$) wave function

$$\begin{aligned} \psi_0(\vec{k}) &= \frac{N(k)}{\sqrt{1 + \frac{1}{4}}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{1}{(k^2 + \frac{1}{4})^2} \quad (1) \quad (2) \\ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{1}{(k^2 + \frac{1}{4})^2} \quad (1) \quad (2) \quad |\vec{k}| < m_1, m_2 \end{aligned} \quad (III.9)$$

$\psi_0(\vec{k}) = \psi_0(\vec{k})$

where $\psi^{(1)}, \psi^{(2)}$ are two-component spinors.

We now examine the Green's function G_0 for kernel K_0 . We require

$$\lim_{\epsilon \rightarrow 0} \left[G_0 = \frac{\psi_0^* \psi_0}{\epsilon - \frac{1}{4}} \right]$$

for second-order perturbation theory Eq. (II.10). Applied to Eq. (III.6a),

the arguments used above lead to a simple relation between G_0 and the non-relativistic Schrodinger-Coulomb propagator:

$$\begin{aligned} G_0(\vec{k}, \vec{q}; \epsilon; m) &= N(k) N(q) G_{Sch}(\vec{k}, \vec{q}; \epsilon; m) \\ G_{Sch}(\vec{k}, \vec{q}; \epsilon; m) & \quad |\vec{k}|, |\vec{q}| < m_1, m_2 \end{aligned} \quad (III.10)$$

Though analytic expressions exist for G_{Sch} in coordinate space,²¹ we find it convenient to use an expression in momentum space due to Schwinger:²²

$$\begin{aligned} G_{Sch}(\vec{k}, \vec{q}; \epsilon; m) &= \frac{(2\pi)^3 \delta^3(\vec{k} - \vec{q})}{\epsilon - \vec{k}^2/2m} - \frac{1}{\epsilon - \vec{k}^2/2m} \frac{e^2}{|\vec{k} - \vec{q}|^2} \frac{1}{\epsilon - \vec{q}^2/2m} \\ &- \frac{e^2}{\epsilon - \vec{k}^2/2m} \int_0^1 d\rho \frac{1}{|\vec{k} - \vec{q}|^2} \frac{1}{\rho - \frac{m}{2\epsilon}} \frac{1}{(\epsilon - \vec{k}^2/2m)(\epsilon - \vec{q}^2/2m)(1 - \rho)^2} \frac{1}{\epsilon - \vec{q}^2/2m} \end{aligned}$$

where $1\eta = \frac{am}{\sqrt{-2m\epsilon}}$. The first two terms are just the zero and one Coulomb terms in the Born series. Integrating by parts and taking $1\eta \rightarrow 1$, we can isolate and remove the ground state pole, and perform the ρ integration.

The resulting (exact) expression is:

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \left[G_{Sch}(\vec{k}, \vec{q}; \epsilon; m) - \frac{\psi_0^*(\vec{k}) \psi_0(\vec{q})}{\epsilon - \frac{1}{4}} \right] &= \frac{64\pi}{a\gamma^4} \left[\frac{\pi^2 \gamma^5 \delta^3(\vec{k} - \vec{q})}{4(k^2 + \gamma^2)} \right. \\ &\left. + \frac{\gamma^6}{4(k^2 + \gamma^2)(\vec{k} - \vec{q})^2(q^2 + \gamma^2)} + \tilde{R}(\vec{k}, \vec{q}) \right] \end{aligned} \quad (III.11a)$$

$\tilde{R}(\vec{k}, \vec{q})$ represents all contributions due to exchange of two or more Coulomb photons and is given by:

$$\begin{aligned} \tilde{R}(\vec{k}, \vec{q}) &= \frac{\gamma^8}{(k^2 + \gamma^2)^2(q^2 + \gamma^2)^2} \left[\frac{5}{2} - \frac{4\gamma^2}{k^2 + \gamma^2} - \frac{4\gamma^2}{q^2 + \gamma^2} \right. \\ &\left. + \frac{1}{2} \ln A + \frac{2A-1}{\sqrt{4A-1}} \tan^{-1} \sqrt{4A-1} \right] \\ A &= \frac{(\vec{k}^2 + \gamma^2)(\vec{q}^2 + \gamma^2)}{4\gamma^2 |\vec{q} - \vec{k}|^2} \end{aligned} \quad (III.11b)$$

For present purposes (i.e., to $O(\alpha^6)$), we need never go beyond second order in perturbation theory. The nature of the perturbations is best understood by combining the expansion in α for G_T with expansions Eqs. (II.3), (II.10) and (III.11). The result to two loops is presented in Fig. 4 in terms of the irreducible BS kernel K_{BS} , the unperturbed kernel $\bar{K}_0$, and $\bar{R}$. The naive order for any kernel in Fig. 4a is α^3 , for the wave function squared, times one α for each photon in the graph. Threshold singularities, if present, increase the contribution over this naive estimate. Examples of singular kernels are the $O(\alpha^5)$ Lamb shift kernels in Fig. 5. These contribute only in $O(\alpha^7)$ to the ground state splitting. Consequently, when computing this splitting to $O(\alpha^6)$, only those parts of K_{BS} need be retained in Fig. 4a as result in diagrams with two or fewer loops. The diagrams in Fig. 4b arise when the dominant static interactions (Fig. 3) are treated in second-order perturbation theory. The leading contribution from these is $O(\alpha^6)$, and has been computed.⁸

C. Decay Rate of Orthopositronium - $O(\alpha)$ Corrections

The decay rate of orthopositronium (n -Ps: $n = 1, J = S = 1$) into three photons is the only annihilation rate of a purely quantum electrodynamic system that has been measured to 1 percent or better (Table I). The most recent theoretical prediction is^{10,11}

$$\begin{aligned} \Gamma_{o-Ps} &= \Gamma^0 \left\{ 1 - \frac{\alpha}{n} 10.266(8) - \frac{1}{3} \alpha^2 \ln \alpha^{-1} + O(\alpha^2) \right\} \\ &= 7.03859(15) \text{ nsec}^{-1} + O(\alpha^8 m_e^{-1} \approx 0.006 \text{ nsec}^{-1}) \end{aligned}$$

Table I
MEASURED DECAY RATE OF ORTHOPOSITRONIUM

<u>Reference</u>	<u>Measured in</u>	<u>Rate (μsec^{-1})</u>
23	Gas	7.056 ± 0.007
24	Gas	7.058 ± 0.015
25	Vacua	7.04 ± 0.02
26	SiO_2 Powder	7.104 ± 0.006
27	Gas	7.262 ± 0.015
28	Gas	7.275 ± 0.015

Experimental determinations of the decay rate of orthopositronium.

$$\begin{aligned}
 & \left((\Pi - \Xi) \times \left[1 + \text{diagram} \frac{\partial}{\partial E} (\Pi - \Xi) \text{diagram} \right] \right) \\
 (a) \quad & \left\{ \begin{aligned} & \text{diagram} - 2 \text{diagram} + \text{diagram} \\ & \text{diagram} - 2 \text{diagram} + \text{diagram} \end{aligned} \right. \\
 (b) \quad & (\Pi - \Xi) \text{diagram} (\Pi - \Xi)
 \end{aligned}$$

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Fig. 4. Kernels contributing to two loops in bound state perturbation theory. The double line represents the BS kernel (Fig. 1).

Fig. 5. Kernels contributing to $\alpha\alpha^5$ Lamb shift and $\alpha\alpha^5$ shifts.

where Γ^0 is the lowest order rate:²⁹

$$\Gamma^0 = \alpha^6 m_e \frac{2(\pi^2 - 9)}{9\pi} = 7.21118 \mu \text{ sec}^{-1}$$

This rate is only just compatible with the most recent measurements and the possibility of a serious discrepancy exists. Although the experimental situation seems far from stable, it is imperative that the theory be examined within the context of a rigorous bound state formalism and all approximations justified. Here we apply the machinery developed in previous sections to this problem. To treat bound states of fermions and anti-fermions, we must replace $u^{(2)}(-\vec{k}, \lambda)$ by $v^{(2)}(-\vec{k}, \lambda)$ in the wave function Eq. (III.5) and in the definitions of $\tilde{\mathcal{O}}$ and $\tilde{\mathcal{K}}$.

The decay of o-Ps occurs via kernels in the perturbation series (Fig. 4), having three-photon intermediate states (Fig. 6a). From Eq. (II.11), the decay rate is simply

$$\begin{aligned} \Gamma &= \int \frac{d^3 \vec{k}}{(2\pi)^3} \frac{d^3 \vec{q}}{(2\pi)^3} \bar{\psi}(\vec{q}) [-2iM(\vec{q}, \vec{k}, P)] \psi(\vec{k}) \\ &= \int \prod_{i=1}^3 \frac{d^3 \vec{k}^{(i)}}{(2\pi)^3 2\omega_i} (2\pi)^4 \delta^4(P - \sum_i k^{(i)}) \left| \int \frac{d^3 \vec{k}}{(2\pi)^3} A(\vec{k}, k^{(i)}) \psi(\vec{k}) \right|^2 \end{aligned} \quad (\text{III.12})$$

Here M is a truncated amplitude describing elastic e^-e^+ scattering, and A is an amplitude describing annihilation into on-shell photons. Amplitude M has an imaginary part because the energy of o-Ps is well above the threshold for producing three photons. The definition of A (Fig. 6b) follows immediately from Fig. 4. All terms contributing through $O(\alpha^2 \Gamma^0)$ to the three-photon decay rate are shown. Five-photon decays also contribute to the total rate at $O(\alpha^2 \Gamma^0)$.

Fig. 6a. The three-photon decay kernel.

Fig. 6b. The three-photon decay amplitude for o-Ps, including all corrections to $O(\alpha^2)$. The double line kernels are two particle irreducible.

The lowest and first-order terms in the decay rate result from the kernels in Fig. 7. Note that we must include propagator corrections on the external fermion legs (Fig. 7c) because they are not on mass-shell. However, the only part of these corrections relevant to $O(\alpha r^0)$ is that which renormalizes the electron charge. It is readily demonstrated that all other contributions from these diagrams (i.e., Fig. 7e) are of $O(\alpha^2 r^0)$ or higher. Thus, we may ignore diagrams (e) in Fig. 7 if we renormalize (a), and (f)-(h) as if they were on-shell amplitudes (the other 1/2 of (e) renormalizes charges in the wave function). The final state photons, being on-shell, are renormalized after the usual fashion.

The only contributions of $O(\alpha r^0)$ from graphs (b) through (i) come from the region of small relative momentum ($k \sim \gamma \ll m_e$) in Eq. (III.12). This is because the decay kernel is approximately independent of $\vec{k}$ (i.e., to $O(k^2/m_e^2) \sim O(r^2)$) when k is nonrelativistic. Of course, the bulk of the wave function is concentrated in this region. Thus, we can replace $A_{b-1}(\vec{k}, k^{(1)})$ by $A_{b-1}(0, k^{(1)})$ in Eq. (III.12) when working only to first order. Furthermore, the effects of binding are negligible here ($O(\alpha^2)$) and therefore, A_{b-1} can be evaluated on mass-shell. The imaginary part of A vanishes below threshold and must be discarded in this approximation. Thus, to leading order, the decay amplitude from graphs (b)-(i) is

$$A_{0-Ps \rightarrow 3\gamma}^{b-i} \approx \int \frac{d^3 k}{(2\pi)^3} \text{Re} A_{b-1}^{MS}(\vec{k}, k^{(1)}) \psi(\vec{k})$$

$$= \text{Re} A_{b-1}^{MS}(0, k^{(1)}) \int \frac{d^3 k}{(2\pi)^3} \psi(\vec{k}) \quad (\text{III.13})$$

Fig. 7. Kernels contributing in lowest and first order to the decay of o-Ps.

The last integral is just the wave function averaged over a volume of radius $\sim 1/m_e$ about the origin in coordinate space, and equals $(\gamma^3/\pi)^{1/2} \times (1 + O(\alpha))$.

An important feature of Eq. (III.13) is that it is completely infrared finite. In Coulomb gauge (used here), infrared divergent terms vanish as $\vec{k}^2/m_e^2$ at threshold in each graph separately. In any gauge, this must be true of the sum of graphs because nonmoving charges cannot radiate in QED. Infrared divergences are cut off in an atom by its size ($\lambda \sim a_0$) and appear as $\ln a_0$'s in the binding energy (e.g., Lamb shift). Their absence here indicates that there are no $O(\alpha^2 \ln \Gamma^0)$ terms arising from these graphs.

Another important feature of Eq. (III.13) is that it is manifestly gauge invariant. This is true (1) because the amplitudes are evaluated on-shell, and (2) because graphs (b) through (i) (excluding the subtraction) form a gauge invariant set. The subtraction term and the wave function involve $\bar{K}_0$ which was defined independently of gauge considerations. Thus, although the analysis above assumed the Coulomb gauge, the actual computations can be carried out in any gauge. In particular we can employ the covariant (and convenient) Feynman gauge.

We turn now to graph (a) in Fig. 7. The leading contribution to the decay rate (Γ^0) comes from (a) when the relative momentum $\vec{k}$ is nonrelativistic:

$$A_{0 \rightarrow P\gamma + 3\gamma}^0 = \int \frac{d^3 \vec{k}}{(2\pi)^3} A_a(\vec{k}, \vec{k}^{(1)}) \psi(\vec{k}) = A_a^{MS}(0, \vec{k}^{(1)}) \int \frac{d^3 \vec{k}}{(2\pi)^3} \psi(\vec{k})$$

$$\rightarrow \Gamma^0 = \frac{1}{\pi} \int \frac{3}{\pi} \int_{i=1}^3 \frac{d^3 \vec{k}^{(i)}}{(2\pi)^3 2\omega_i} (2\pi)^4 \delta^4(P - \sum \vec{k}^{(i)}) \left| \frac{\bar{v}(0) A_a^{MS}(0, \vec{k}^{(1)}) u(0)}{2m_e} \right|^2$$

The only other contributions from this region of $\vec{k}$ -space are of $O(\alpha^2 \Gamma^0)$. This follows from the analyticity of $M_a(\vec{k}, \vec{q})$ (Eq. (III.12)) in $\vec{k}$ and $\vec{q}$ which implies:

$$M_a(\vec{k}, \vec{q}) = M_a(0, 0) \left[1 + O\left(\frac{\vec{k}^2}{m_e^2}, \frac{\vec{q}^2}{m_e^2}, \frac{(\vec{k} \cdot \vec{q})}{m_e^2}\right) \right]$$

$$= M_a(0, 0) [1 + O(\alpha^2)] \quad (\text{III.14})$$

The amplitude is analytic because its branch points occur when $s = 0$ or $t = 4m_e^2$ - both far from the region we are considering ($s \sim 4m_e^2$, $t \sim 0$). Therefore, the only contributions of $O(\alpha \Gamma^0)$ from this graph arise from the relativistic region of $\vec{k}$ -space.

To further analyse the graph we use the bound state equations (Eq. (III.4)) to iterate the wave function (Fig. 8a). We can then compare this term to the subtraction in (b) evaluated on-shell as in Eq. (III.13). The two should cancel, at least in leading order (Fig. 8b). They differ only in that the total energy (appearing in the k -integration loop) is $P^0 = 2m_e - \alpha^2 m_e/4$ in the first and $P = 2\sqrt{\vec{q}^2 + m_e^2} = 2m_e + \vec{q}^2/m_e^2$ in the second. In each case only $\vec{q}$ of $O(\gamma)$ contribute. When $\vec{k}$ is relativistic, $O(\alpha^2)$ corrections to the propagators are irrelevant (e.g., $s^{-1} = P^0 - 2E(k) = 2(m_e - E(k)) = O(m_e)^{-1}$). In this region the graphs cancel. When $\vec{k}$ is non-relativistic, the decay amplitude $A_a(\vec{k} \rightarrow 0, \vec{k}^{(1)})$ factors out. If then we approximate the propagator $s^{-1} = P^0 - 2E(k) \sim P^0 - 2m_e - \frac{\vec{k}^2}{2m_e}$, the

difference between the two terms is

$$\begin{aligned}
 & - \frac{\bar{v}(0) A_{d-i}^{MS}(0, k^{(1)}) u(0)}{2m_e} \left(\frac{\gamma}{\pi} \right)^{1/2} \operatorname{Re} \left[\int \frac{d^3 k}{(2\pi)^3} \int \frac{d^3 q}{(2\pi)^3} \frac{8\pi\gamma}{(q^2 + \gamma^2)^2} \frac{1}{k^2 - q^2} \right. \\
 & \quad \left. \times \left(\frac{m}{k^2 + \gamma^2} - \frac{m}{k^2 - q^2} \right) + O(a^2) \right] \\
 & = - \frac{\bar{v} A_{d-i}^{MS} u}{2m_e} \left(\frac{\gamma}{\pi} \right)^{1/2} \operatorname{Re} \left[\frac{8\pi\gamma}{(2\pi)^6} \int \frac{d^3 k}{k^2 + \gamma^2} \int \frac{d^3 q}{q^2 + \gamma^2} \frac{1}{|k - q|^2} \frac{1}{k^2 - q^2} + O(a^2) \right] \\
 & = 0
 \end{aligned}$$

by symmetry. Thus, graph (a) in Fig. 7 is completely cancelled to $O(a^0)$ by the subtraction term in (b), even when the latter is evaluated on-shell. Consequently, graphs (a), (b) and (c) may be replaced by the real part of (c') evaluated on-shell (Fig. 7). Graph (c') is identical to (c) but with a complete photon propagator in place of the transverse propagator. Now, relativistic wave function momenta in graph (a) appear as relativistic loop momenta in (c').

The entire decay amplitude, including all radiative corrections of $O(a)$, can now be written in terms of gauge invariant on-shell amplitudes, and a nonrelativistic wave function:

$$A_{0-Ps \rightarrow \gamma}(k^{(1)}) = \int \frac{d^3 k}{(2\pi)^3} \operatorname{Re} \left[A_{c'}^{MS}(k, k^{(1)}) \phi(k) + \left(\frac{\gamma}{\pi} \right)^{1/2} \frac{\bar{v}(0) A_{d-i}^{MS}(0, k^{(1)}) u(0)}{2m_e} \right]$$

The computation of these terms is described in Refs. 10 and 11. The results are listed in Table II. We also list the results of Strosio and Holt,³⁰ the first to attempt the $O(a^0)$ calculation (note their sign error

Fig. 8a. Iteration of the wave function.

Fig. 8b. Cancellation between iteration of graph in Fig. 7a, and the subtraction in Fig. 7b evaluated on-shell.

Table II

O(α) CORRECTIONS TO THE DECAY RATE OF ORTHOPOSITRONIUM

	Caswell, Lepage and Saperstein ^{10,11}	Strosio and Holt ³⁰
Γ_d	-0.809 ± 0.004	-0.5 ± 0.2
Γ_f	$4.791 \pm 0.003 + 4\ln(\lambda/m_e)$	$4.785 \pm 0.010 + 4\ln(\lambda/m_e)$
$\Gamma_{g,h}$	$-2.868 \pm 0.003 - 6\ln(\lambda/m_e)$	$-2.8716 \pm 0.0036 - 6\ln(\lambda/m_e)$
Γ_i	-3.562 ± 0.004	-3.355 ± 0.003
$\Gamma_{c'}^{IR}$	$-2 + 2\ln(\lambda/m_e)$	$-2 + 2\ln(\lambda/m_e)$
$\Gamma_{c'}^S$	-5.818 ± 0.008	5.8 ± 0.4
Total	-10.266 ± 0.008	1.86 ± 0.45

Theoretical determinations of the O(α) corrections to the decay rate of orthopositronium (in units of $(\alpha/\pi)\Gamma^0$). $\Gamma_d = -0.741 \pm 0.017$ is quoted in Ref. 31.

in $\Gamma_{c'}$. Spurious infrared divergences appear because the calculation was done in Feynman gauge. As expected these cancel in the final answer. Graph (c') has both a logarithmic singularity and a $1/|q|$ singularity at threshold. These are removed by subtracting

$$A_{c'}^{IR} = \text{Re} \left[ie^2 \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 - \lambda^2} \frac{1}{k^2 + 2P_1 \cdot k} \frac{1}{k^2 - 2P_2 \cdot k} \right] 4m_e^2 A_a^{MS}(k=0, k^{(i)})$$

$$= \frac{\alpha}{2\pi} \left[2 \ln\left(\frac{\lambda}{m_e}\right) + \frac{\pi^2 m_e}{|q|} - 2 \right] A_a^{MS}(k=0, k^{(i)})$$

from $A_{c'}$, where $P_1 = \frac{p}{2} + q$ and $P_2 = \frac{p}{2} - q$. This amplitude when convoluted with the wave function contributes

$$\Gamma_{c'}^{IR} = \Gamma^0 + \left[2 \ln\left(\frac{\lambda}{m_e}\right) - 2 \right] \frac{\alpha}{\pi} \Gamma^0$$

The singular $1/q$ part of $A_{c'}^{IR}$ gave rise to the leading order term. The subtracted rate was found to be

$$\Gamma_{c'}^S = -5.818(S) \frac{\alpha}{\pi} \Gamma^0$$

The total rate from c' is the sum $\Gamma_{c'}^{IR} + \Gamma_{c'}^S$.

The method described above for expressing O(α) correction in terms of Schroedinger wave functions and gauge invariant on-shell amplitudes is applicable to many other problems. As an example we cite the calculation of O(α) corrections to the hyperfine splitting of the ground state in positronium (or muonium). The procedure described here is considerably simpler than the BS analysis originally employed by Karplus and Klein.³²

D. Decay Rate of Orthopositronium $\propto (\alpha^2/m_e^{-1})$ Corrections

In this section we compute the $O(\alpha^2/m_e^{-1})$ corrections to the decay rate of o-Ps. These are potentially the largest of all second order corrections ($\alpha^2/m_e^{-1} \sim 5$) though in fact the coefficient turns out to be small.

The diagrams considered and their contributions are presented in Fig. 9. For all these diagrams it is found that α^2/m_e^{-1} terms come only from the region of nonrelativistic momenta in all loop integrations (excluding integrations over final states). Only there are the fermion propagators in the kernel sufficiently singular for the binding energy to be of any importance. Thus, the general procedure to be adopted is to expand all energies $E(k)$ and propagators in powers of k^2/m_e^2 and then to isolate terms which diverge logarithmically. These are the source of α^2/m_e^{-1} contributions. Of course the divergences are ultimately cut off by the propagators at momenta of $O(m_e)$. At the lower end, the cut off is due to the finite size of the atom ($k \sim (\text{Bohr radius})^{-1} \sim O(\alpha)$) and binding effects. The coefficient of α^2/m_e^{-1} is easily computed using Table III.

In the nonrelativistic region, each graph contributes terms only of $O(\alpha^2/m_e^0)$ or higher. Consequently the amplitude in each case can be approximated by

$$A_{\text{o-Ps} \rightarrow \gamma \gamma} = \int \frac{d^3q_1 d^3q_2 d^3q_3}{(2\pi)^9} \frac{v(q_1) A_{\gamma\gamma}(q_1, k^{(1)}) u(q_2)}{2m_e} \frac{G^{(0)}(q_1, p_1; q_2, p_2; q_3, k)}{i(p_1 - q_1) i(p_2 - q_2) i(k - q_3)}$$

where δK is any of the leading instantaneous perturbation kernels

(Eq. (III.8), Fig. 1) and $G^{(0),1}$ represents the nonrelativistic propagator with either zero or one Coulomb interaction:

$$G^{(0)} = \frac{(2\pi)^3 \delta(\vec{q} - \vec{p})}{i(p - q/m_e)} \quad G^{(1)} = \frac{1}{i(p - q/m_e)} \frac{1}{i(p - q/m_e)} \frac{1}{i(p - q/m_e)} \frac{1}{i(p - q/m_e)} \frac{1}{i(p - q/m_e)} \frac{1}{i(p - q/m_e)}$$

Table III

TABLE OF INTEGRALS

$$\int_{\text{non}} \frac{d^3k}{k^4} \frac{d^3q}{q^4} \frac{f(k, q)}{|\vec{k} - \vec{q}|^2} = K \pi^4 \ln \alpha^{-1}$$

$f(k, q)$	K
$1, q^4$	0
$k^2 q^2$	4
$k^2 k \cdot q, q^2 k \cdot q$	2
$(k \cdot q)^2$	2

Table of integrals required for analytic evaluations.

Ag: in $A_a(q, k^{(k)})$ can be replaced by $A_a^{MS}(0, k^{(1)})$ and we find that each graph in Fig. 9 contributes

$$\Gamma = 2\Gamma^0 \int \frac{d^3k}{(2\pi)^3} \frac{8\pi\gamma}{(k^2 + \gamma^2)^2} \int \frac{d^3q d^3p}{(2\pi)^6} \left\langle G^{0,1}(q, p, \epsilon) i \delta \vec{k} (\vec{p} - \vec{k}, \epsilon) \right\rangle_{\epsilon=0} \quad (III.15)$$

to the decay rate. We examine each term separately:

(a) Coulomb Correction: Combining δK_C^0 (Eq. (III.8a)) with G^0 we obtain the contribution from diagram (a) in Fig. 9:

$$\begin{aligned} \Gamma_a &= 2\Gamma^0 \frac{\gamma}{\pi^2} \int \frac{d^3k}{(k^2 + \gamma^2)^2} \int \frac{d^3q}{q^2 + \gamma^2} \frac{-m_e}{|\vec{k} - \vec{q}|^2} \left\{ \frac{4\vec{k} \cdot \vec{q} - \vec{q}^2 - \vec{k}^2}{8m_e^2} - \frac{\gamma^2}{8} \right\} \\ &= \Gamma^0 \frac{\alpha^2}{16\pi^4} \int \frac{d^3k}{(k^2 + \gamma^2)^2} \int \frac{d^3q}{q^2 + \gamma^2} \frac{4\vec{k} \cdot \vec{q} - \vec{q}^2 - \vec{k}^2 - \alpha^2 \pi_e^2}{|\vec{k} - \vec{q}|^2} \end{aligned}$$

Terms in δK_C^0 proportional to $\vec{k} \times \vec{q} \cdot \vec{\sigma}$ integrate to zero because the wave function is symmetric. The terms $4\vec{k} \cdot \vec{q}$ and $-\vec{k}^2$ in the numerator lead to logarithmic divergences. From Table III we find immediately:

$$\Gamma_a = \frac{1}{4} \alpha^2 \ln \alpha^{-1} \Gamma^0 + O(\alpha^2 \Gamma^0)$$

Diagram (b) in Fig. 9 is identical to (a) but with G^0 replaced by G^1 :

$$\begin{aligned} \Gamma_b &= 2\Gamma^0 \frac{\gamma}{\pi^2} \int \frac{d^3k}{(k^2 + \gamma^2)^2} \int \frac{d^3q d^3p}{(2\pi)^6} \frac{-m_e}{q^2 + \gamma^2} \frac{-e^2}{|\vec{q} - \vec{p}|^2} \frac{-m_e}{p^2 + \gamma^2} \frac{-e^2}{|\vec{k} - \vec{p}|^2} \\ &\times \left\{ \frac{4\vec{k} \cdot \vec{p} - \vec{k}^2 - \vec{p}^2 - \alpha^2 m_e^2}{|\vec{k} - \vec{p}|^2} \right\} \end{aligned}$$

KERNEL	COEFFICIENT OF $\alpha^2 \ln \alpha^{-1} \Gamma^0$
(a)	$\frac{1}{4}$
(b)	$-\frac{1}{4}$
(c)	1
(d)	$-\frac{1}{3}$
(e)	-1
5-78 J40349 TOTAL	$-\frac{1}{3}$

Fig. 9. Diagrams contributing to $O(\alpha^2 \ln \alpha^{-1} \Gamma^0)$ in o-PS decay.

Only the $\vec{p}^2$ term diverges logarithmically. We find

$$\begin{aligned} \Gamma_b &= \Gamma^0 \frac{\alpha^2}{16\pi^4} \left(\frac{\gamma}{\pi^2} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \right) \int \frac{d^3 q}{\vec{q}^2 + \gamma^2} \frac{d^3 p}{\vec{p}^2 + \gamma^2} \frac{1}{|\vec{q} - \vec{p}|} \frac{\vec{p}^2}{|\vec{p}|^2} \\ &= -\frac{1}{4} \alpha^2 \ln \alpha^{-1} \Gamma^0 + O(\alpha^2 \Gamma^0) \end{aligned}$$

(b) Transverse Photon: The calculation for diagrams (c) and (d) is analogous to that just described-- $\delta \hat{K}_I$ (Eq. (III.8b)) replaces $\delta \hat{K}_C$. Note that in the o-PS state $\langle \vec{\sigma}_1 \cdot \vec{\sigma}_2 \rangle_{J=S=1} = 1$. The diagrams contribute

$$\begin{aligned} \Gamma_c &= -\Gamma^0 \frac{\alpha^2}{2\pi^4} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \int \frac{d^3 q}{\vec{q}^2 + \gamma^2} \frac{1}{|\vec{k} - \vec{q}|^2} \left\{ \frac{(\vec{k} \cdot \vec{q})^2 - \vec{k}^2 \vec{q}^2}{|\vec{k} - \vec{q}|^2} + \frac{|\vec{k} - \vec{q}|^2}{6} \right\} \\ &= \alpha^2 \ln \alpha^{-1} \Gamma^0 + O(\alpha^2 \Gamma^0) \\ \Gamma_d &= -\Gamma^0 \frac{\alpha^2}{2\pi^4} \frac{\gamma}{\pi^2} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \int \frac{d^3 q}{\vec{q}^2 + \gamma^2} \frac{d^3 p}{\vec{p}^2 + \gamma^2} \frac{1}{|\vec{q} - \vec{p}|^2} \frac{1}{|\vec{k} - \vec{p}|^2} \\ &\quad \times \left\{ \frac{(\vec{k} \cdot \vec{p})^2 - \vec{k}^2 \vec{p}^2}{|\vec{k} - \vec{p}|^2} + \frac{|\vec{k} - \vec{p}|^2}{6} \right\} \\ &= -\Gamma^0 \frac{\alpha^2}{12\pi^4} \left(\frac{\gamma}{\pi^2} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \right) \int \frac{d^3 q}{\vec{q}^2 + \gamma^2} \frac{d^3 p}{\vec{p}^2 + \gamma^2} \frac{1}{|\vec{q} - \vec{p}|^2} \\ &= -\frac{1}{3} \alpha^2 \ln \alpha^{-1} \Gamma^0 + O(\alpha^2 \Gamma^0) \end{aligned}$$

(c) Annihilation to One Photon: When $\delta \hat{K}_A$ is combined with $G^{(1)}$ in Eq. (III.15) the result diverges linearly. This indicates an $O(\alpha \Gamma^0)$ contribution from the relativistic region (as computed earlier), but no terms of $O(\alpha^2 \ln \alpha^{-1} \Gamma^0)$. Only with $G^{(1)}$ does $\delta \hat{K}_A$ contribute (Fig. 9e):

$$\begin{aligned} \Gamma_e &= -\Gamma^0 \frac{\alpha^2}{4\pi^4} \frac{\gamma}{\pi^2} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \int \frac{d^3 q}{\vec{q}^2 + \gamma^2} \frac{d^3 p}{\vec{p}^2 + \gamma^2} \frac{1}{|\vec{q} - \vec{p}|^2} \\ &= -\alpha^2 \ln \alpha^{-1} \Gamma^0 + O(\alpha^2 \Gamma^0) \end{aligned}$$

The only other kernels which might be sufficiently singular to contain $\alpha^2 \ln \alpha^{-1}$ corrections are the lowest order decay kernel (Fig. 7a), and the terms just considered but with two or more intermediate Coulomb interactions (i.e., last term in Fig. 6b). The first, though, contributes to $O(\alpha^2 \Gamma^0)$, results in no $\ln \alpha^{-1}$ terms. This is readily demonstrated given expansion Eq. (III.14). Contributions from the second source have been computed numerically using expression Eq. (III.11) for $\hat{K}$. The analytic results quoted for these in Fig. 10 agree to five figures (at least) with the numerical results. No further $\ln \alpha^{-1}$ terms appear here.

IV. A DIRAC EQUATION FOR AN EFFECTIVE PARTICLE

A. Introduction

In this section we discuss a bound state equation for the BS wave function with one constituent on its mass-shell. This formalism originated with Gross¹³ and has subsequently been discussed by several authors.^{14,9} The major attraction of this formulation is that in ladder approximation it reduces to the Dirac-Coulomb equation when the mass of the on-shell constituent is taken to infinity. This is very desirable when studying atoms whose constituents differ greatly in mass. However, the asymmetric treatment of the constituents is less desirable when they are equal in mass. Thus, although the treatment is completely general, we shall only apply it here to atoms having a large mass ratio (e.g., muonium). It is usually more convenient to use the formalism described in Section III when the mass ratio is arbitrary or near unity.

Gross' suggestion is to replace the RS propagator by

$$S(k, p) = 2 - i \frac{(k^2 - m_1^2)^{(1)} \dots (k^2 - m_l^2)^{(1)}}{(p^2 - k^2 - m_1^2)^{(2)}} \quad (IV.1)$$

The two-particle Green's function satisfies an equation

$$\bar{G}(\vec{k}, \vec{q}, P) = - \frac{(\vec{k} + m_1)(\vec{q})}{(P - \vec{k} - m_2)(\vec{q})} \left\{ \frac{1}{(1 - \vec{k} - \vec{q})^2} \frac{1}{k^2} (\vec{k} - \vec{q}) + \int \frac{d^4 l}{(2\pi)^4} \frac{1}{l^2} \frac{1}{k^2} \frac{1}{(l + \vec{k} - \vec{q})^2} \bar{G}(\vec{l}, \vec{q}, P) \right\} \\ \frac{1}{k^2} \left\{ \frac{1}{k^2} + m_1^2 \right\} \quad (IV, 2)$$

$$= \frac{i}{p^0 - p_n^0} \frac{n(k) - n(q)}{n} \quad \text{as } p^0 \rightarrow p_n^0$$

where the truncated part of $\bar{G}$ is related to the complete four-point function (Eq. (II.2)) by

$$\bar{G}_T(\vec{k} \vec{q} P) = \lim_{\substack{k^0 \rightarrow E_k \\ q^0 \rightarrow E_q}} i G_T(k q P)$$

The various poles and cuts of K_{BS} are reintroduced into $\bar{K}$ by definition (Eq. (II.3)):

$$\bar{K}(k q P) = K_{BS}(k q P) \Big|_{k^0=E_k, q^0=E_q}$$

$$+ \int \frac{d^4 r}{(2\pi)^4} K_{BS}(k r P) \frac{i}{(r^2 - m_2^2)^{(2)}}$$

$$\times \left\{ \frac{i}{(r^2 - m_1^2)^{(1)}} - 2\pi \delta^+(r^2 - m_1^2) (r^2 + m_1^2)^{(1)} \right\} K_{BS}(r q P) \Big|_{k^0=E_k, q^0=E_q}$$

+ ...

On physical grounds we expect the first term to dominate when the binding is weak or when $m_1 \gg m_2$. In either case particle one remains close to its mass-shell.

The bound state equations follow immediately from Eq. (IV.2):

$$(\not{P} - \not{K} - m_2)^{(2)} \psi(\vec{k}) = (\not{K} + m_1)^{(1)} \int \frac{d^3 k}{2E_k (2\pi)^3} i K(\vec{k} \vec{q} P) \psi(\vec{q})$$

$$(\not{K} - m_1)^{(1)} \psi(\vec{k}) = 0$$

$$k^0 = E_k$$

The second of these equations implies that

$$\psi(\vec{k}) = \sum_{\lambda=1}^2 \sqrt{2E_k} u^{(1)}(\vec{k} \lambda) \cdot \chi(\vec{k}) \quad (IV.3)$$

where $u^{(1)}$ is an on-shell spinor and $\cdot$ has eight components--four spinor components for particle two and two spin components for particle one. Wave function χ satisfies

$$(\not{P} - \not{K} - m_2) \psi(\vec{k}) = \int \frac{d^3 q}{(2\pi)^3} i \tilde{K}(\vec{k} \vec{q} P) \psi(\vec{q}) \quad (IV.4a)$$

where

$$\tilde{K}(\vec{k} \vec{q} P)_{\lambda\lambda'} = \frac{\bar{u}^{(1)}(\vec{k} \lambda) \bar{K}(k q P) u^{(1)}(\vec{q} \lambda')}{\sqrt{4E_k E_q}} \quad (IV.4b)$$

It is normalized as in Eq. (II.8) with weight function

$$W(\vec{k} \vec{q} P, P_n) = \gamma_0 [(2\pi)^3 \delta^3(\vec{k} - \vec{q})]$$

$$= \frac{i \tilde{K}(\vec{k} \vec{q} P)_m - i \tilde{K}(\vec{k} \vec{q} P)_n}{P_m^0 - P_n^0}$$

Again, perturbation theory (Section II.B) can be expressed in terms of ψ , $\bar{G}$ and $\bar{K}$ or in terms of ψ , $\tilde{K}$ and $\tilde{G}$ (defined analogously to $\tilde{K}$).

One advantage of this approach is its partial gauge invariance which occurs because m_1 propagates on-shell. By current conservation, this formalism is invariant under the general class of gauge transformations

$$= \frac{g_{\mu\nu}}{k^2} \rightarrow - \frac{R_{\mu\nu} + f(k, A) k_\mu A_\nu}{k^2}$$

performed upon all photons interacting with m_1 (index μ) and, in particular, on all photons in simple ladder and cross-ladder kernels. Unfortunately, this class of gauges does not include the Coulomb gauge, though in general any gauge-dependent terms associated with these photon lines must vanish in the Dirac limit ($m_1 \rightarrow \infty$).

B. The Unperturbed QED Problem

Here we solve Eq. (IV.4) with a kernel $\tilde{K}_0$ which approximates the QED interaction. The solutions are exact in $Z\alpha$ and correct to lowest and first order in m_2/m_1 . This is sufficiently accurate for all calculations in muonium and hydrogen. These solutions are also correct to all orders in m_2/m_1 in the nonrelativistic limit ($\frac{k}{m_2} \sim Z\alpha \rightarrow 0$). Another solution is described in Ref. 9 which is exact to all orders in m_2/m_1 but somewhat less convenient to use.

We first rewrite Eq. (IV.4):

$$(P - E_k + \vec{\alpha} \cdot \vec{k} - \beta m_2) \psi(\vec{k}) - \int \frac{d^3 q}{(2\pi)^3} V(\vec{k}, \vec{q}) \psi(\vec{q}) = 0$$

that is

$$(P^0 - E_k + \vec{\alpha} \cdot \vec{k} - \beta m_2 - V) \psi = 0 \quad (IV.5a)$$

where

$$V(\vec{k}, \vec{q}) \equiv \gamma^0 \tilde{K}(\vec{k}, \vec{q}) \quad (IV.5b)$$

Equation (IV.5) is greatly complicated by the term $E_k = \sqrt{k^2 + m_1^2}$. Grotch and Yennie,³⁵ employing a similar equation, expanded E_k to first order in k^2/m_1^2 , but this procedure leads to anomalous divergences in the $O(\alpha^2 m_2/m_1)$ corrections. To remove E_k , we multiply by $(P^0 + E_k + \vec{\alpha} \cdot \vec{k} - \beta m_2 - V)/2P^0$ to obtain

$$\left\{ E' + \vec{\alpha} \cdot \vec{k} - \beta m_2 - V + \frac{V^2}{2P^0} - \left\{ V, \frac{\vec{\alpha} \cdot \vec{k}}{2P^0} \right\} + \left\{ \frac{\beta m_2}{2P^0}, V \right\} \right. \\ \left. + \left[V, \frac{E_k}{2P^0} \right] \right\} \psi = 0 \quad (IV.6)$$

where

$$E' = \frac{P^0 + m_2^2 - m_1^2}{2P^0} = m_2 + \epsilon + \frac{m_1^2}{P^0} + \frac{V^2}{2P^0}$$

and $\epsilon = P^0 - m_1 - m_2$. The potential due to one-photon exchange (Coulomb and transverse) is

$$V_{\perp V}(\vec{k}, \vec{q}) = \frac{-Ze^2}{\vec{k} - \vec{q}} \left(1 + \frac{i\vec{k} \cdot \vec{q} + \vec{q} \cdot \vec{q}}{4m_1^2} \right) + \frac{Ze^2}{2m_1} \left(\frac{\vec{\alpha} \cdot (\vec{k} + \vec{q})}{\vec{k} - \vec{q}} \right. \\ \left. - \frac{\vec{\alpha} \cdot (\vec{k} - \vec{q})(\vec{k}^2 - \vec{q}^2)}{\vec{k} - \vec{q}} + \frac{i(\vec{q} - \vec{k}) \cdot \vec{\alpha} \cdot (\vec{k} + \vec{q})}{(\vec{k} - \vec{q})^2} \right) \quad (IV.7)$$

It is responsible for all the binding energy up to and including $O((Z\alpha)^4)$.

We approximate this potential by

$$V_0(\vec{k}, \vec{q}) = \frac{-Ze^2}{(\vec{k} - \vec{q})^2} + \frac{Ze^2}{2m_1} \frac{\vec{\alpha} \cdot (\vec{k} + \vec{q})}{(\vec{k} - \vec{q})^2} + \frac{Ze^2 P^0}{16m_1^2 (\vec{k} - \vec{q})^2} \\ \left(-\frac{2V}{r} + \left[\frac{2\alpha}{r} + \frac{\vec{\alpha} \cdot \vec{k}}{2m_1} \right] + \frac{\alpha^2}{2m_1 r^2} \text{ in coordinate space} \right) \quad (IV.8)$$

This is just the Dirac equation for a single effective particle moving in an external Coulomb field. The spectrum is well known:

$$\frac{E}{m} = \left[1 + \frac{(c^2 + \frac{1}{2} \frac{d^2}{dt^2})^2}{(c^2 + \frac{1}{2} \frac{d^2}{dt^2})^2 + c^4} \right]^{1/2}$$

$$= 1 + \frac{1}{m} + \frac{1}{2m_1 m_2}$$

$$= -\frac{(73)^2}{24} = -(73)^2 = -\begin{pmatrix} 1 & 1 & 1 & 1 \\ 20 & 14 & 20 & 14 \\ 14 & 20 & 14 & 20 \\ 20 & 14 & 20 & 14 \end{pmatrix}$$

$$+ O((m_1)^4 - m^3, m_1^2) \quad n = n' + 1 + \dots$$

Aside from hyperfine terms, this is the complete spectrum to $O(\hbar^2/m_1)$.

The (normalized) wave functions are just the usual Dirac-Coulomb wave functions $\psi_{n+1}^{(2)}(-\vec{k})$:

$$\psi(\vec{k}) = \begin{pmatrix} 1 + i \\ 1 + i \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 1 \end{pmatrix} \cdot (-\vec{k}) \cdot (1) \quad (IV.14)$$

with $Z_{\alpha, m}$ replaced by $Z_{\alpha, m}^*$. We require the ground state wave function in the next section:

$$g_{15}^{(2)} = g_{\text{O}}^{(2)}(-\vec{k}) + g_{\text{II}}^{(2)}(-\vec{k}) + g_{\text{L}}^{(2)}(-\vec{k})$$

[illegible]

$$\delta\phi_{\text{L}}^{(2)}(-\vec{k}) = \left(\frac{\gamma}{\pi}\right)^{\frac{1}{2}} \frac{8\pi\gamma}{(k^2 + \gamma^2)^2} \frac{(Z\alpha)^2}{4} \\ \times \left\{ \ln\left(\frac{\gamma^2 + \vec{k}^2}{\gamma^2}\right) + \frac{\vec{k}^2 - \gamma^2}{k\gamma} \tan^{-1} \frac{k}{\gamma} \right\} \begin{bmatrix} \chi^{(2)} \\ 0 \end{bmatrix} \\ + \left\{ \frac{\gamma^2 + 2\vec{k}^2}{\gamma^2} + \ln\left(\frac{\gamma^2 + \vec{k}^2}{\gamma^2}\right) - \frac{3\vec{k}^2\gamma + \gamma^3}{k^3} \tan^{-1} \frac{k}{\gamma} \right\} \begin{bmatrix} 0 \\ -\frac{\vec{\sigma} \cdot \vec{k}}{2m} \chi^{(2)} \end{bmatrix}$$

where

$$\gamma = Z\alpha\tilde{m} = Z\alpha\tilde{m} (1 + O((Z\alpha)^2)) \quad (\text{IV.12})$$

$$N = 1 + \left(\frac{1}{4} - \ln 2\right) (Z\alpha)^2/2 + O((Z\alpha)^4)$$

Note that $\delta\phi$ is $O((Z\alpha)^2\phi_0)$ when $k \sim O(\gamma)$, and $O(Z\alpha\phi_0)$ when $\vec{k}$ is relativistic ($\sim m$).

As indicated above, the only perturbations of $O((Z\alpha)^4)$ are in $V_{1\gamma} - V_0$ (Eqs. (IV.7,8)):

$$i\delta\tilde{K}_{1\gamma}(\vec{k}, \vec{q}) = \gamma^0 (V_{1\gamma} - V_0)$$

$$= -\frac{Ze^2}{2m_1} \frac{\vec{\gamma} \cdot (\vec{k} - \vec{q}) (k^2 - q^2)}{|\vec{k} - \vec{q}|^4} - \frac{Ze^4 \gamma^0}{16m_1 |\vec{k} - \vec{q}|} \\ + \frac{Ze^2}{2m_1} \frac{1(\vec{q} - \vec{k}) \times \vec{\sigma}_1 \cdot \vec{\gamma}}{|\vec{k} - \vec{q}|^2} - \frac{Ze^2}{4m_1^2} \gamma^0 \frac{1 \vec{k} \times \vec{q} \cdot \vec{\sigma}_1}{|\vec{k} - \vec{q}|^2} \quad (\text{IV.13})$$

KERNEL

COEFFICIENT OF

$$\alpha^2 \frac{m_e}{m_\mu} \ln \alpha^{-1} E_F$$

(a) $\frac{1}{4}$

(b) $\frac{5}{2}$

(c) $-\frac{3}{4}$

(d) $2 \left[\text{box with cross on top} + \text{box with cross on bottom} - \text{box with cross on both} \right] = 0$
TOTAL $\frac{0}{2}$

(e) $\bar{K}_0 = \text{box with cross on top} + \text{box with cross on bottom}$ 3401811

Fig. 11. Kernels contributing to $O(\alpha^2 m_e/m_\mu \ln \alpha^{-1} E_F)$ in muonium hfs. An 'x' on a fermion line indicates that it is on mass-shell.

Although the diagonal matrix elements of the first two terms cancel, the off-diagonal elements are of $O((Z\alpha)^4 m^2/m_1)$. Consequently, these terms are as important as the hyperfine interaction when we consider contributions from second-order perturbation theory in the next section.

C. Muonium Hyperfine Splitting to $O(\alpha^6 \ln \alpha^{-1})$

Here we compute all $O(\alpha^6 \ln \alpha^{-1})$ contributions to the ground state hyperfine splitting (hfs) in muonium ($e^- \mu^+$). The current theoretical estimate of the hfs is³⁷

$$\Delta E_{\mu e} = E_F \left[\frac{1}{\mu_0(u)} (1 + a_e + \frac{3}{2} \alpha^2 - \frac{1}{2} \alpha^2 - \ln 2) \right. \\ \left. + \frac{\mu}{\mu_0(u)} \frac{m_e}{m_\mu} \left(-\frac{3a}{\pi} \frac{\ln(m_\mu/m_e)}{1 - (m_e/m_\mu)^2} + \frac{2\alpha^2 \ln \alpha^{-1}}{(1 + m_e/m_\mu)^2} + O(\alpha^2) \right) \right. \\ \left. + \frac{\alpha^3}{\pi} \left(-\frac{2}{3} \ln^2 \alpha^{-2} + \left(\frac{37}{72} + \frac{4}{15} - \frac{8}{3} \ln 2 \right) + (18.36 \pm 5) \right) \right] \quad (IV.14)$$

where a_e is the electron's anomalous magnetic moment and E_F is the "Fermi Splitting":

$$E_F = \frac{2}{3} \frac{\alpha m}{m_e m_\mu} \left\langle \vec{\sigma}_e \cdot \vec{\sigma}_\mu \right\rangle \Big|_{J=0} = \frac{8}{3} \frac{\alpha m}{m_e m_\mu}$$

Current experimental results are sensitive to all terms exhibited as well as the many $O(\alpha^2 m_e/m_\mu E_F, \alpha^3 E_F)$ terms not yet computed.

The diagrams contributing to $O(\alpha^2 m_e/m_\mu \ln \alpha^{-1} E_F)$ are presented in Fig. 11 (cf. Fig. 4). The procedure for isolating $\ln \alpha$'s is as described in Section III.D--that is, expand all energies and propagators in powers

of k^2/m_e^2 and seek out $O(\alpha^2 m_e/m_\mu \ln \alpha^{-1})$ terms which appear to diverge logarithmically. We examine each contribution in turn:

(a) One-Photon Corrections (Fig. 11a): Two terms in $\delta E_{1\gamma}$ (Eq. IV.13) contribute to the hfs. The first comes from exchange of a transverse photon:

$$\delta E_{\gamma_1} = \int \frac{d^3 k}{(2\pi)^3} \int \frac{d^3 q}{(2\pi)^3} \bar{\psi}(\vec{k}) \gamma^4 \psi(\vec{q}) \frac{i e^2 (\vec{q} - \vec{k}) \times \vec{\sigma}_\mu}{2m_\mu |\vec{k} - \vec{q}|^2}$$

The contributions from δ_0 and $\delta\phi$, respectively, are

$$\delta E_{\gamma_1} = \delta E_0 + \delta E_1$$

$$\delta E_0 = \frac{\gamma^5}{\pi} \frac{\alpha N^2}{m_\mu m_e} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \frac{d^3 q}{(\vec{q}^2 + \gamma^2)^2} \frac{(\vec{k} - \vec{q}) \times \vec{\sigma}_e \cdot (\vec{k} - \vec{q}) \times \vec{\sigma}_\mu}{|\vec{k} - \vec{q}|^2}$$

$$= E_F$$

$$\delta E_1 = \frac{\gamma^5 \alpha^3}{2\pi m_e m_\mu} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \frac{d^3 q}{(\vec{q}^2 + \gamma^2)^2} \left[-\frac{\vec{q} \times \vec{\sigma}_e \cdot (\vec{k} - \vec{q}) \times \vec{\sigma}_\mu}{|\vec{k} - \vec{q}|^2} \left\{ \ln \left(\frac{\gamma^2 + \vec{k}^2}{\gamma^2} \right) \right. \right. \\ \left. \left. + \frac{\vec{k}^2 - \gamma^2}{k\gamma} \tan^{-1} \frac{k}{\gamma} + \frac{\vec{k} \times \vec{\sigma}_e \cdot (\vec{k} - \vec{q}) \times \vec{\sigma}_\mu}{|\vec{k} - \vec{q}|^2} \left\{ \frac{\gamma^2 + 2\vec{k}^2}{\vec{k}^2} \right. \right. \right. \\ \left. \left. + \ln \left(\frac{\gamma^2 + \vec{k}^2}{\gamma^2} \right) - \frac{3\vec{k}^2}{k^3} + \frac{\gamma^3}{k} \tan^{-1} \frac{k}{\gamma} \right\} \right]$$

The "Fermi splitting" is contained in δE_0 , but no $\alpha^2 \ln \alpha^{-1}$ terms. In δE_1 we can rescale all momenta by γ . The result is a convergent integral

independent of α . There are no $\alpha^2 \ln \alpha^{-1}$ terms here.

The other relevant term in δK_{1Y} comes from the Coulomb interaction (the lower spinor components):⁵

$$\begin{aligned} \delta E_{Yc} &= -\frac{e^2}{4m_\mu^2} \int \frac{d^3 k}{(2\pi)^6} \frac{d^3 q}{6} \bar{\psi}(\vec{k}) \gamma^0 \psi(\vec{q}) \frac{1}{|\vec{k}-\vec{q}|^2} \frac{\vec{k} \times \vec{q} \cdot \vec{\sigma}_\mu}{|\vec{k}-\vec{q}|^2} \\ &= +\frac{E_F}{8\pi} \alpha^2 \frac{m_e}{m_\mu} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \frac{d^3 q}{(\vec{q}^2 + \gamma^2)^2} \frac{|\vec{k} \times \vec{q}|^2}{|\vec{k}-\vec{q}|^2} \end{aligned}$$

This integral diverges logarithmically. The factors $E_k, E_q, \dots$ cut it off at m_μ while it is cut off at the lower end by $\gamma \approx \alpha m_e$. Referring to Table III we find

$$\begin{aligned} \delta E_{Yc} &= +\frac{1}{4} \alpha^2 \frac{m_e}{m_\mu} \ln \alpha^{-1} E_F + \frac{1}{4} \alpha^2 \frac{m_e}{m_\mu} \ln \frac{m_\mu}{m_e} E_F \\ &+ O(\alpha^2 \frac{m_e}{m_\mu} E_F) \end{aligned}$$

which is δE_a in Fig. 11.

(b) Two-Transverse Photons (Fig. 11b): The contributions from the ladder and cross-ladder diagrams with two transverse photons have been computed and are described in the literature.³⁸ The result is $\frac{9}{2} \alpha^2 m_e/m_\mu \ln \alpha^{-1} E_F$. However, parts of the interaction due to exchange of a transverse photon are already in K_0 and are, therefore, included to all orders in the wave function. To avoid double counting (of parts of δE_a) these must be removed, as indicated in Fig. 11b. Here we compute the

subtraction:

$$\begin{aligned} \delta E_{TT}^S &= -\frac{2e^4}{4m_\mu^2} \int \frac{d^3 k}{(2\pi)^9} \frac{d^3 q}{2} \frac{d^3 r}{E_r} \bar{\psi}(\vec{r}) \left(\vec{\gamma} \cdot \frac{i(\vec{r}-\vec{k}) \times \vec{\sigma}_\mu}{|\vec{r}-\vec{k}|^2} \right) \frac{1}{\vec{r}^2 - \vec{k}^2 - m_e^2} \\ &\times \left(\vec{\gamma} \cdot \frac{(\vec{r}+\vec{q})}{|\vec{r}-\vec{q}|^2} + \frac{\pi \gamma^0}{2|\vec{r}-\vec{q}|} \right) \psi(\vec{q}) \Big|_{r^0 = E_r} \\ &= E_F \frac{\gamma \alpha^2}{2\pi^6} \frac{m_e}{m_\mu} \int \frac{d^3 k}{(\vec{k}^2 + \gamma^2)^2} \frac{d^3 q}{(\vec{q}^2 + \gamma^2)^2} \frac{d^3 r}{\vec{r}^2 + \gamma^2} \frac{1}{|\vec{r}-\vec{k}|^2} \\ &\times \left\{ |\vec{r}-\vec{k}|^2 \left(-\frac{(\vec{r}+\vec{q})^2}{|\vec{r}-\vec{q}|^2} + \frac{\pi \gamma}{|\vec{r}-\vec{q}|} \right) - \frac{(\vec{r}^2 + \gamma^2)(\vec{r}-\vec{k}) \cdot (\vec{r}+\vec{q})}{|\vec{r}-\vec{q}|^2} \right\} \end{aligned}$$

We have replaced ψ by $\psi^{(2)}$ and $(\vec{r}-\vec{r})^2 - m_e^2$ by $-(\vec{r}^2 + \gamma^2)$. Isolating just the divergent terms:

$$\begin{aligned} \delta E_{TT}^S &= \frac{1}{2} E_F \alpha^2 \frac{m_e}{m_\mu} \left[\frac{1}{4} \int \frac{d^3 q}{(\vec{q}^2 + \gamma^2)^2} \frac{d^3 r}{\vec{r}^2 + \gamma^2} \frac{2\vec{r} \cdot \vec{q} - \vec{q}^2}{|\vec{r}-\vec{q}|^2} + \frac{1}{\pi} \int \frac{d^3 r}{\vec{r}(\vec{r}^2 + \gamma^2)} \right] \\ &= 2 E_F \alpha^2 \frac{m_e}{m_\mu} \ln \alpha^{-1} + O(\alpha^2 \frac{m_e}{m_\mu} E_F) \end{aligned}$$

Combining this with the known contribution from the complete ladder and cross-ladder diagrams we obtain

$$\delta E_b = \frac{5}{2} \alpha^2 \frac{m_e}{m_\mu} \ln \alpha^{-1} E_F + O(\alpha^2 \frac{m_e}{m_\mu} E_F)$$

(c) Two-Transverse, One-Coulomb Photons (Fig. 11c): Again the contribution from this diagram with complete transverse photons has been computed,^{39,9} and the result is $\frac{5}{4} \alpha^2 m_e/m_\mu \ln \alpha^{-1} E_F$. From this we must remove the iterations of lower order results. The subtraction term to be added here is

$$\delta E_{TCT}^S = \frac{2e^6}{4m_\mu^2} \int \frac{d^3k}{(2\pi)^6} \frac{d^3q}{(2\pi)^6} \frac{d^3r}{(2\pi)^6} \frac{d^3p}{(2\pi)^6} \bar{\psi}(\vec{k}) \left(\vec{\gamma} \cdot \frac{1(\vec{r}-\vec{k}) \times \vec{\sigma}}{|\vec{r}-\vec{k}|^2} \right) \\ \times \frac{1}{\vec{p}-\vec{r}-m_e} \frac{\gamma^0}{|\vec{r}-\vec{p}|^2} \frac{1}{\vec{p}-\vec{r}-m_e} \left(\frac{\vec{\gamma} \cdot (\vec{p}+\vec{q})}{|\vec{p}-\vec{q}|^2} + \frac{\pi \alpha \gamma^0}{2|\vec{p}-\vec{q}|} \right) \psi(\vec{q})$$

This integral diverges only when the integrations over k and q factor-- i.e., when set $k, q \sim \gamma \sim 0$ in the kernel. The only divergent term is

$$\delta E_{TCT}^S = -\frac{E_F}{2\pi} \alpha^2 \frac{m_e}{m_\mu} \int_{-\infty}^{\infty} \frac{d^3r}{r^2 + \gamma^2} \frac{d^3p}{p^2 + \gamma^2} \frac{1}{|\vec{p}-\vec{r}|^2} \\ = -2 \alpha^2 \frac{m_e}{m_\mu} \ln \alpha^{-1} E_F + O(\alpha^2 \frac{m_e}{m_\mu} E_F)$$

Thus the total contribution from graphs (c) in Fig. 11 is

$$\delta E_C = -\frac{3}{4} \alpha^2 \frac{m_e}{m_\mu} \ln \alpha^{-1} E_F + O(\alpha^2 \frac{m_e}{m_\mu} E_F)$$

(d) One-Transverse, One-Coulomb Photons (Fig. 11d): The first two diagrams in Fig. 11d are most conveniently computed by closing the integration contour for the loop energy at infinity thereby encircling the poles

in the propagators--the muon, photon and positron poles in the ladder diagram; the antimuon, photon and positron poles in the cross-ladder. The contribution from the ladder diagram's muon pole has already been included (in δE_A) and must be omitted. This leaves only terms from the photon poles in each diagram; antiparticle poles correspond to "Z-graphs" in time-ordered perturbation and are not sufficiently singular to contribute. However, $O(\alpha^2 \ln \alpha^{-1} E_F)$ contributions from the photon pole term in the ladder diagram have been shown to completely cancel those from the cross-ladder.⁹ Hence, there is no contribution from graphs (d) in Fig. 11.

The diagrams in Fig. 12 appear to contribute to order $\alpha^2 \ln \alpha^{-1} E_F$ (no factor m_e/m_μ , as above). In fact, it is trivially shown that these terms exactly cancel to this order in pairs as indicated in Fig. 12. Note also that intermediate multi-Coulomb exchange in diagrams such as Fig. 11c leads to $O(\alpha^2 m_e/m_\mu E_F)$ terms, but no $\ln \alpha$'s (see Ref. 8).

The total $O(\alpha^2 m_e/m_\mu \ln \alpha^{-1} E_F)$ hyperfine splitting of the muonium ground state is

$$\delta E_{a-d} = 2 \alpha^2 \frac{m_e}{m_\mu} \ln \alpha^{-1} E_F \\ = 0.0112 \text{ MHz}$$

This result has recently been confirmed by Bodwin and Yennie.²⁰ Theory and experiment are compared in Table IV. Little can be said about the comparison at least until all terms of the form $\alpha^2 m_e/m_\mu (\ln m_\mu/m_e)^n E_F$ have been computed.

D. Positronium Ground State Splitting to $O(\alpha^6 \ln \alpha^{-1})$

The current theoretical estimate of the ground state splitting in

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Fig. 12. Diagrams which cancel pairwise to $O(\alpha^2 m_e/m_\mu \ln \alpha^{-1} E_F)$.
An 'x' on a line indicates that it is on mass-shell.

Table IV

THEORY AND EXPERIMENT - MUONIUM HFS.

Theory

$$E_F + O\left(\alpha \frac{m_e}{m_\mu} E_F, \alpha^2 E_F, \alpha^3 E_F\right) \quad 4463.293 (6) \text{ MHz}$$

$$2\pi^2 \frac{m_e}{m_\mu} E_F \ln \alpha^{-1} \quad 0.011$$

$$\text{Total Theory} \quad 4463.304 (6) \text{ MHz}$$

Experiment

$$\text{Ref. 3} \quad 4463.30235 (52) \text{ MHz}$$

Comparison of theory and experiment for muonium hfs.

Uncertainties shown in theory due to uncertainties in m_e/m_μ (Ref. 3). Terms of $O(\alpha^2 m_e/m_\mu \ln m_e/m_\mu E_F) \sim 0.01$ MHz have yet to be computed and are not included.

positronium is³⁷

$$\Delta E_{ee} = E_F \left(\frac{\mu_e}{\mu_0} \right)^2 \left[1 - \frac{3}{2} \frac{\alpha}{\pi} + \frac{\alpha^2 \ln \alpha^{-1}}{2} + O(\alpha^2) \right] \\ + E_A \left[1 - \frac{2\alpha}{\pi} \left(\frac{13}{9} + \ln^2 \right) + \frac{\alpha^2 \ln \alpha^{-1}}{6} + O(\alpha^2) \right]$$

where the Fermi splitting in positronium is

$$E_F = \frac{\alpha^4 m_e}{3}$$

and E_A is the splitting due to annihilation into one photon (Fig. 3c):

$$E_A = \frac{\alpha^4 m_e}{4}$$

The first term in ΔE is just the muonium result Eq. (IV.14) with $m_\mu \rightarrow m_e$.

In particular, the calculations of $O(\alpha^2 m_e/m_\mu \ln \alpha^{-1} E_F)$ discussed above have been carried out to all orders in m_e/m_μ using the formalism described above.⁹

The exact mass dependence is that exhibited in Eq. (IV.14).

The second term in ΔE is due to one- and two-photon annihilation kernels and is peculiar to positronium. The terms of this sort contributing to $O(\alpha^2 \ln \alpha^{-1} E_A)$ are exhibited in Fig. 13. These can be evaluated immediately (using the formalism described in Section III) by noting that 1) they are identical in form to the three-photon annihilation graphs discussed in Section III.D (Fig. 9) but with one photon replacing three; and 2) like the three-photon annihilation kernel, the one-photon annihilation kernel (Fig. 3c) is essentially momentum independent for nonrelativistic momenta and factors out of the calculation. Thus, we need only replace Γ^0 by E_A

Fig. 13. Contributions of $O(\alpha^2 \ln \alpha^{-1} E_A)$ to the positronium ground state splitting coming from annihilation graphs. These are computed using the formalism described in Section III.

in the expressions generated in Section III.B, being careful not to count diagram (g) in Fig. 13 twice. The final result is (some of these contributions were first presented in Refs. 39, 40)

$$\delta E_{e-g} = \frac{\alpha^2 \ln \alpha^{-1}}{6} E_F$$

Combining this with the contribution from ladder graphs we obtain the total $O(\alpha^6 m_e \ln \alpha^{-1})$ ground state splitting for positronium:

$$\begin{aligned} \delta E_{a-g} &= \alpha^2 \ln \alpha^{-1} \left(\frac{E_F}{2} + \frac{E_A}{6} \right) = \frac{5}{24} \alpha^6 \ln \alpha^{-1} m_e \\ &= 0.0191 \text{ GHz} \end{aligned}$$

Again, theory and experiment (Table V) are consistent within errors. However, the comparison will not be satisfactory until all $O(\alpha^6 m_e)$ terms have been computed.

Table V

THEORY AND EXPERIMENT - POSITRONIUM Hfs.

Theory

$O(\alpha^4 m_e, \alpha^5 m_e)$	203.3812 GHz
$\frac{5}{24} \alpha^6 m_e \ln \alpha^{-1}$	0.0191
Total Theory	203.4003 GHz

Experiment

Ref. 1	203.3849 (12) GHz
Ref. 2	203.3870 (16) GHz

Comparison of theory and experiment for positronium hfs. Terms of $O(\alpha^2 m_e/2) \approx 0.01$ GHz are not yet computed.

V. CONCLUSIONS

Evaluation of the entire $O(\alpha^6)$ ground state splitting in muonium and positronium is among the most important remaining high order QED calculations. This calculation is straightforward using the methods described above, and much of it is amenable to computer analysis since

- 1) simple analytic expressions exist for the unperturbed wave functions;
- 2) corrections to the unperturbed binding energies are unambiguously specified in perturbation theory;
- 3) spinor algebra can be performed automatically.

It is likely that bound state calculations can be systematized to the same extent as (g-2) calculations.

Of the $O(\alpha^6)$ terms, the only ones that have been computed to date are:

- all $O(\alpha^6 \ln \alpha^{-1})$ contributions (Section IV);
- all terms requiring a Bethe-type sum-over-states (Fig. 4b)⁸;
- all terms in positronium involving annihilation into two or three photons.⁴¹

A large but finite number of kernels having two loops or fewer remains to be considered (Fig. 4a). An added complication is that calculations should be carried out in the Coulomb gauge for the reasons discussed in Section IIC.

For muonium it is also necessary to compute all terms of $O(\alpha^3 E_F \sim \alpha^7 m_e^2/m_\mu)$. Since recoil corrections (i.e., $O(\alpha^3 m_e/m_\mu E_F)$) are irrelevant here, this part of the calculation can be done using the Dirac equation for an electron in an external field (i.e., $m_e/m_\mu \rightarrow 0$ in Section IV). The leading terms have already been computed;⁴² evaluation of the remainder is again straightforward though involved.

Each kernel contributing to $O(\alpha^6)$ in muonium also contributes in positronium--here the only difference between the atoms is the mass ratio, m_2/m_1 . Of course, for positronium there are additional annihilation kernels. Calculations for both atoms can be carried out simultaneously using the formalism of Section III. This formalism is well suited to the study of nonrelativistic atoms, such as these, having any ratio m_2/m_1 .

The theoretical analysis of the decay rate of orthopositronium is similar to that of the ground-state splitting. The current status of this analysis is also the same--there remains a large number of decay kernels having two loops or fewer which contribute to $O(\alpha^2 \Gamma^0)$ (Fig. 6b). The relative importance of higher order corrections is somewhat enhanced here since the lowest order rate has an anomalously small numerical coefficient ($\Gamma^0 \sim \alpha^6 m_e/16$). The coefficient in higher order terms need not be so small and indeed it is not for the $O(\alpha^0)$ corrections. Even accounting for this enhancement, experimental errors must be reduced by at least an order of magnitude before the decay rate measurement is as stringent a test of theory as the measurement of ground state splittings. Still, this is the only annihilation decay whose rate is known both theoretically and experimentally with an accuracy of $\sim 0.1\%$.

The only other accurately determined property of a pure QED atom is the $^3S_1 - ^3P_2$ splitting in positronium. Theory and experiment are in agreement:

$$\text{Theory: } ^{43} \quad E = 8629.14 \text{ MHz} \pm 0.2 \text{ MHz}$$

$$\text{Experiment: } ^{44} \quad \Delta E = (8629.4 \pm 2.8) \text{ MHz}$$

Again $O(\alpha^2)$ corrections have yet to be computed.

As discussed earlier, the techniques developed in Section IV are very

well suited to analyses where only lowest and first orders in m_2/m_1 are important. They can be useful in verifying the $O(\alpha^6)$ hfs in muonium. This formalism should also be quite useful in the analysis of nuclear recoil effects in hydrogen atoms or in high Z atoms. In addition, both the formalism and that described in Section III have applications in the analysis of non-QED atoms--e.g., relativistic analysis of the spectra of ψ/J , D, U, ... mesons.

To summarize, we find that the theory of pure QED systems is generally in accord with experiment, though less precise. There appear to be no problems of principle in refining theoretical predictions.

REFERENCES

1. P. O. Egan, W. E. Frieze, V. W. Hughes and M. H. Yam, Phys. Lett. 54A, 412 (1975).
2. A. P. Mills, Jr. and G. H. Berman, Phys. Rev. Lett. 34, 246 (1975).
3. D. E. Casperson, T. W. Crane, A. B. Denison, P. O. Egan, V. W. Hughes, F. G. Mariam, H. Orth, H. W. Reist, P. A. Souder, R. D. Stambaugh, P. A. Thompson, and G. Zupulitz, Phys. Rev. Lett. 38, 956 (1977).
4. Y. Nambu, Prog. of Theor. Phys. 5, 614 (1950); J. Schwinger, Proc. Nat. Acad. Sci. U.S. 37, 452 (1951); E. E. Salpeter and H. A. Bethe, Phys. Rev. 84, 1232 (1951); see also review by S. J. Brodsky, "Lectures on Atomic Physics and Astrophysics," in Atomic Physics and Astrophysics Vol. K, ed. M. Chretien and E. Lipworth (Gordon and Breach, N.Y., 1969).
5. Note however, the wavefunctions discussed in Sections III and IV are also solutions of the BS equation. Thus, it is now possible, though still awkward, to use the BS formalism. Also, progress has been made in generating approximate solutions which are sufficiently accurate to compute $O(\alpha^2)$ corrections to hfs: V. K. Cung, T. Fulton, W. W. Repko, and D. Schnitzler, Ann. Phys. (N.Y.) 96, 261 (1976); V. K. Cung, T. Fulton, W. W. Repko, A. Schaum, and D. Devoro, Ann. Phys. (N.Y.) 98, 516 (1976).
6. E. E. Salpeter, Phys. Rev. 87, 328 (1952).
7. The method for accomplishing this transformation (see Section II.1) has been rediscovered many times. See, for example: A. A. Logunov and A. N. Tavkhelidze, Nuovo Cim. 29, 380 (1963); R. Blankenbecler

- and R. Sugar, Phys. Rev. 142, 1051 (1966); A. Klein and T. H. Lee, Phys. Rev. D10, 4308 (1974).
8. W. E. Caswell and G. P. Lepage, SLAC-PUB-2080, Feb. 1978.
  9. G. P. Lepage, Phys. Rev. A16, 863 (1977).
  10. W. E. Caswell, G. P. Lepage and J. Saperstein, Phys. Rev. Lett. 38, 488 (1977).
  11. W. E. Caswell and G. P. Lepage, in preparation.
  12. A. Messiah, Quantum Mechanics, Vol. II (John Wiley & Sons, New York, 1962), Section 16.15.
  13. There are nonexponential terms in the decay probability due to the decay channel's branch cut. These are negligible in general and are ignored here. They are discussed in M. L. Goldberger and K. M. Watson, Collision Theory, Chapter 8 (Kreiger, Huntington, N.Y., 1975).
  14. G. Breit, Phys. Rev. 34, 553 (1929).
  15. We thank S. Love for several conversations concerning these terms.
  16. R. N. Faustov, Sov. J. of Particles and Nuclei 3, 119 (1972) [Fizika Elementarnykh Chastits i Atomnogo Yadra 3, 238 (1972)].
  17. This choice of k^0 and q^0 results in constituent energies

$$E_1 = \gamma_1 P_0 \quad E_2 = \gamma_2 P_0$$

This is but one of many possible alternatives. Another is

$$E_1 = \frac{P_0^2 - m_2^2 + m_1^2}{2P_0} \quad E_2 = \frac{P_0^2 - m_1^2 + m_2^2}{2P_0}$$

which is symmetric in the masses and which restricts the constituents to their mass shell when P_0 is above threshold. Thus, $\bar{G}$ becomes the usual scattering amplitude when $P_0 \geq m_1 + m_2$. This last property also

follows when one constituent is put on its mass shell

$$E_1 = \sqrt{k^2 + m_1^2} \quad E_2 = P_0 - E_1$$

This choice also results in a limited form of gauge invariance (see Section IV.1). None of the results of this paper is altered if either of these alternatives is adopted.

18. It is conceivable that the residue vanishes and thus $\bar{G}$ may contain fewer bound states than G_T . This is not the case for nonrelativistic QED systems.
19. The truncated wavefunctions (i.e., $(P_0 - E_1 - E_2)\psi$) obtained in this formalism for kernel $\bar{K}(\vec{k}, \vec{q}, P)$ are (truncated) wave functions of the BS equation with kernel $\Lambda_+^{(1)}(\vec{k}) \Lambda_+^{(2)}(-\vec{k}) \gamma_0^{(1)} \gamma_0^{(2)} \times \bar{K}(\vec{k}, \vec{q}, P) \Lambda_+^{(1)}(\vec{q}) \Lambda_+^{(2)}(-\vec{q})$.
20. This method of rationalizing the propagator is suggested in G. T. Bodwin and D. R. Yennie, "Hyperfine Structure in Positronium and Muonium," Cornell preprint CLNS-383 (Dec. 1977), to be published in Phys. Rep.
21. E. H. Wichmann and C. H. Woo, J. Math. Phys. 2, 178 (1961); L. Hostler, J. Math. Phys. 5, 591 (1964).
22. J. Schwinger, M. Math. Phys. 5, 1601 (1964).
23. D. W. Gidley, A. Rich, P. W. Zitzewitz and D.A.L. Paul, Phys. Rev. Lett. 40, 737 (1978).
24. T. C. Griffith and G. R. Heyland, Nature 269, 109 (1977).
25. D. W. Gidley, P. W. Zitzewitz, K. A. Marko, and A. Rich, Phys. Rev. Lett. 37, 729 (1976).
26. D. W. Gidley, K. A. Marko, and A. Rich, Phys. Rev. Lett. 36, 395 (1976).

27. P. G. Coleman and T. C. Griffith, J. Phys. B 6, 2155 (1973).
28. V. W. Hughes, Physik 1973, Plenarvortrag Physikertagung 37th
(Physik Verlag, Weinheim, Germany, 1973), pp. 123-155 (in English).
29. A. Ore and J. L. Powell, Phys. Rev. 75, 1696 (1949).
30. M. A. Strosio and J. M. Holt, Phys. Rev. A10, 749 (1974);
M. A. Strosio, Phys. Rep. 22C, 217 (1974).
31. P. Pascual and E. deRafael, Lett. Nuovo Cim. 4, 1144 (1970).
32. R. Karplus and A. Klein, Phys. Rev. 87, 848 (1952).
33. F. Gross, Phys. Rev. 186, 1448 (1969).
34. C. Fronsdal and R. W. Huff, Phys. Rev. D3, 933 (1971). S. J.
Brodsky, in Proc. 3rd Colloquium on Advanced Computing Methods
in Theoretical Physics, Marseilles, 1973; L. S. Duljan and R. N.
Faustov, "Modified Dirac Equation in Quantum Field Theory,"
Joint Institute of Nuclear Research preprint P2-7995, Dubna,
1974 (in Russian).
35. H. Grotch and D. R. Yennie, Rev. Mod. Phys. 41, 350 (1969).
36. The term $[E_k, V]/2P^0 \sim (E_k - E_q)/|\vec{k} - \vec{q}|^2$ in momentum space contributes
nothing in 1st order perturbation theory because it is antisymmetric
in k and q . In 2nd order it contributes at most $O(\alpha^6 m_e^4/m_\mu^3)$ and so
may safely be omitted. Certain other terms omitted are, in fact,
too singular at $r=0$ to be treated in perturbation theory (e.g.,
 $\alpha^4/8m_1^3 r^4$). These singularities can be avoided by restricting
 $|\vec{k} - \vec{q}| \lesssim m_1$ (i.e., $r \lesssim 1/m_1$) in the last two terms of V_0 (Eq. (IV.8)).
Then all terms omitted from Eq. (IV.9) are calculable and negligible
(i.e., $O((m_2/m_1)^2)$).
37. B. E. Lautrup, A. Peterman, and E. deRafael, Phys. Rep. 3, 193 (1972).

38. T. Fulton, D. A. Owen, and W. W. Repko, Phys. Rev. A4, 1802 (1971).
39. R. Barbieri and E. Remiddi, Phys. Lett. 65B, 258 (1976).
40. D. A. Owen, Phys. Rev. Lett. 30, 887 (1973).
41. V. K. Cung, A. Devoto, T. Fulton and W. W. Repko, Phys. Lett.
68B, 474 (1977), and Michigan State University preprint (March 1978).
42. S. J. Brodsky and G. W. Erickson, Phys. Rev. 148, 26 (1966); A. J.
Layzer, Nuovo Cim. 33, 1538 (1964); D. E. Zwanziger, Nuovo Cim. 34,
77 (1964).
43. T. Fulton and P. C. Martin, Phys. Rev. 95, 811 (1954).
44. A. P. Mills, Jr., S. Barko and K. F. Canter, Phys. Rev. Lett. 34,
177 (1975).

27. P. G. Coleman and T. C. Griffith, J. Phys. B 6, 2155 (1973).
28. V. W. Hughes, Physik 1973, Plenarvortrag Physikertagung 37th
(Physik Verlag, Weinheim, Germany, 1973), pp. 123-155 (in English).
29. A. Ore and J. L. Powell, Phys. Rev. 75, 1696 (1949).
30. M. A. Strosio and J. M. Holt, Phys. Rev. A10, 749 (1974);
M. A. Strosio, Phys. Rep. 22C, 217 (1974).
31. P. Pascual and E. deRafael, Lett. Nuovo Cim. 4, 1144 (1970).
32. R. Karplus and A. Klein, Phys. Rev. 87, 848 (1952).
33. F. Gross, Phys. Rev. 186, 1448 (1969).
34. C. Fronsdal and R. W. Huff, Phys. Rev. D3, 933 (1971). S. J.
Brodsky, in Proc. 3rd Colloquium on Advanced Computing Methods
in Theoretical Physics, Marseilles, 1973; L. S. Duljan and R. N.
Faustov, "Modified Dirac Equation in Quantum Field Theory,"
Joint Institute of Nuclear Research preprint P2-7995, Dubna,
1974 (in Russian).
35. H. Grotch and D. R. Yennie, Rev. Mod. Phys. 41, 350 (1969).
36. The term $[E_k, V]/2P^0 \sim (E_k - E_q)/|\vec{k} - \vec{q}|^2$ in momentum space contributes
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37. B. E. Lautrup, A. Peterman, and E. deRafael, Phys. Rep. 3, 193 (1972).

38. T. Fulton, D. A. Owen, and W. W. Repko, Phys. Rev. A4, 1802 (1971).
39. R. Barbieri and E. Remiddi, Phys. Lett. 65B, 258 (1976).
40. D. A. Owen, Phys. Rev. Lett. 30, 887 (1973).
41. V. K. Cung, A. Devoto, T. Fulton and W. W. Repko, Phys. Lett.
68B, 474 (1977), and Michigan State University preprint (March 1978).
42. S. J. Brodsky and G. W. Erickson, Phys. Rev. 148, 26 (1966); A. J.
Layzer, Nuovo Cim. 33, 1538 (1964); D. E. Zwanziger, Nuovo Cim. 34,
77 (1964).
43. T. Fulton and P. C. Martin, Phys. Rev. 95, 811 (1954).
44. A. P. Mills, Jr., S. Barko and K. F. Canter, Phys. Rev. Lett. 34,
177 (1975).