Relativistic corrections to the Zeeman effect in hydrogenlike atoms and positronium

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An approximately relativistic theory of bound states which ensures Poincaré invariance of the atomic system to relative order $(v/c)^2$ developed by one of us [K. J. Sebastian, Phys. Rev. A **23**, 2810 (1981)] is used to derive the Zeeman interaction Hamiltonian for a two-body system. This Hamiltonian is correct to order $\alpha(Z\alpha)^2$ and to all orders of m_e/m_N and includes contributions from previously neglected radiative and recoil corrections. Explicit analytic expressions for the g_J and g_I factors are given and verify the results of Grotch and Kashuba [Phys. Rev. A **7**, 78 (1973)]. This interaction Hamiltonian in conjunction with the zero-field relativistic interaction correct to order $\alpha(Z\alpha)^4$ is used to analyze the Zeeman structure of the $n = 1, 2$, and 3 levels of hydrogen and positronium. In the case of hydrogen, corrections for the Lamb shift which include the most recent radiative recoil and pure recoil corrections have also been included to yield an extremely precise analysis for hydrogen in the $|nFm_FJL\rangle$ representation. The Hamiltonian, g factors, and Zeeman splittings are compared with previously obtained results and experimental results. The results of these comparisons are discussed at length.

I. INTRODUCTION

The past two decades have witnessed significant advances in the experimental determination of the energy levels of one-electron atoms and positronium. The measurement of the fine structure and the hyperfine structure of atomic hydrogen [1] and positronium [2–5] and the measurement of the Lamb shifts in atomic hydrogen [6–8] all require the use of a constant external magnetic field for their determination. To interpret these results a precise understanding of the Zeeman effect in hydrogenlike atoms and positronium is essential. Attempts in this direction have been made in the past [9–14]. In Ref. [10] the minimally substituted Breit equation was reduced to a Schrödinger-Pauli form to obtain the linear Zeeman Hamiltonian which is almost correct to order $\alpha(Z\alpha)^2$ and to all orders in m_e/m_N for hydrogenlike atoms, where α is the fine-structure constant, Z is the atomic number, and m_e and m_N are the electronic and nuclear masses, respectively. In Refs. [9] and [12] the minimally substituted Breit equation was reduced to a Schrödinger-Pauli form to obtain the linear Zeeman Hamiltonian which is correct to order α^3 for positronium. The results of Refs. [9–12] are correct only for neutral systems. Faustov [13] used a different approach to obtain the g factors of hydrogen correct to order $\alpha(Z\alpha)^2(m_e/m_N)^2$ and $\alpha(Z\alpha)^2(m_e/m_N)$. Close and Osborn [14] utilized an approach which ensures Poincaré invariance of the atomic system to order $(v/c)^2$ to obtain the g factors for the 1S state of hydrogen correct to order $\alpha(Z\alpha)^2$ and to all orders in m_e/m_N.

However, their approach is distinctly different from the approach used here. The authors of all of the above works neglected radiative corrections of order $\alpha(Z\alpha)^2(m_e/m_N)^q$ ($q = 0, 1, \ldots, \infty$) and recoil corrections of order $\alpha(Z\alpha)^2(m_e/m_N)^q$ ($q = 1, \ldots, \infty$).

We will calculate the relativistic corrections to the Zeeman effect in hydrogenlike atoms and positronium using an approximately relativistic theory of bound states which was developed by one of us (K.J.S.) [15–18] and is based upon the work of Foldy [19], Bakamjian and Thomas [20], and others [21]. The basic idea here is to make the Hilbert space of the composite system a reducible representation of the Poincaré group to relative order $(1/c)^2$. The results presented here are correct to $\alpha(Z\alpha)^2$ and to all orders in m_e/m_N.

In Sec. II we derive the linear Zeeman Hamiltonians for hydrogenlike atoms of arbitrary atomic number and positronium. The Hamiltonian for hydrogenlike atoms contains previously neglected radiative contributions which were first obtained by Grotch and Kashuba [9] and recoil corrections resulting from the exchange of a single transverse photon between the electron and the nucleus when the atom is in a constant external magnetic field. These corrections are proportional to L_z and are of minor importance for the $L \neq 0$ states. However, they do not contribute to the positronium Hamiltonian. For neutral systems our Hamiltonian, which describes a composite system in an external uniform magnetic field (B), can be obtained by a unitary transformation of the Hamiltonian of Grotch and Hegstrom [10] [Eq. (40) of Ref. [10]] to first order in B. For systems with a net electric charge ($Z \neq 1$) there are additional contributions of order $(Z\alpha)^2 m_e/m_N$ and $\alpha(Z\alpha)^2 m_e/m_N$ in our Hamiltonian beyond those in the Hamiltonians of Grotch and Kashuba [9] and of Grotch and Hegstrom [10].

In Sec. III the g_I and g_J factors for hydrogenlike atoms with nuclear spin $\frac{1}{2}$ are obtained. When an expansion is made in terms of α, m_e/m_N, and ε (the nonrelativistic binding energy) the results of Grotch and Kashuba [9] for the g_I and g_J factors for hydrogenlike atoms of nuclear spin 1/2 are verified. Our g_J factor includes a contribu-

tion (g'_J) from the previously neglected radiative and recoil corrections.

In Sec. IV a g factor for the ground state of positronium is obtained. This g factor agrees exactly with the g factor obtained by Grotch and Kashuba [9] and Lewis and Hughes [12].

In Sec. V the linear Zeeman Hamiltonian, the relativistic internal Hamiltonian correct to order $\alpha(Z\alpha)^4$, and the lowest-order quadratic Zeeman Hamiltonian are used in degenerate perturbation theory to solve for the energy eigenvalues as a function of the magnetic field for the $n=1$, 2, and 3, levels of hydrogen and positronium. A concise summary of the paper is presented in Sec. VI.

II. THE INTERACTION HAMILTONIAN

The total Hamiltonian for the isolated composite system of two constituent particles can be written to order $1/c^2$ as

$$H = \sum_{\mu=1}^{2} \left[\frac{p_\mu^2}{2m_\mu} - \frac{P_\mu^4}{8m_\mu^3 c^2} \right] + U^{(0)} + U^{(1)} , \qquad (1)$$

where p_μ is the constituent momentum of the μth particle and $U^{(0)}$ and $U^{(1)}$ are the internal interactions of the zeroth and second order in v/c, respectively. For two-body atomic systems $U^{(0)}$ is the Coulomb interaction between the two particles and $U^{(1)}$ is given primarily by the Fermi-Breit interaction [21,22]

$$U_{FB}^{(1)} = \frac{Ze^2}{2m_1 m_2 c^2} \left\{ \left[\mathbf{p}_1 \frac{1}{q} \cdot \mathbf{p}_2 + \mathbf{p}_1 \cdot \mathbf{q} \frac{1}{q^3} \mathbf{q} \cdot \mathbf{p}_2 \right] - 2(1+a_1)\mathbf{s}_1 \cdot \left[\frac{\mathbf{q}}{q^3} \times \mathbf{p}_2 \right] \right.$$

$$+ 2(1+a_2)\mathbf{s}_2 \left[\frac{\mathbf{q}}{q^3} \times \mathbf{p}_1 \right] - \frac{m_1}{m_2}(1+2a_2)\mathbf{s}_2 \cdot \left[\frac{\mathbf{q}}{q^3} \times \mathbf{p}_2 \right] + \frac{m_2}{m_1}(1+2a_1)\mathbf{s}_1 \cdot \left[\frac{\mathbf{q}}{q^3} \times \mathbf{p}_1 \right]$$

$$+ \left[\frac{m_1}{m_2}(1+2a_2) + \frac{m_2}{m_1}(1+2a_1) \right] \pi \delta^{(3)}(\mathbf{q})$$

$$\left. - (1+a_1)(1+a_2) \left[\frac{\mathbf{s}_1 \cdot \mathbf{s}_2}{q^3} - \frac{3(\mathbf{s}_1 \cdot \mathbf{q})(\mathbf{s}_2 \cdot \mathbf{q})}{q^5} - \frac{8}{3}\pi(\mathbf{s}_1 \cdot \mathbf{s}_2)\delta^{(3)}(\mathbf{q}) \right] \right\} , \qquad (2)$$

where $\mathbf{s}_1, \mathbf{s}_2$; $\mathbf{p}_1, \mathbf{p}_2$; and a_1, a_2 are the spins, momenta, and anomalous magnetic moment parameters of the two particles, respectively. With the position vectors of the two particles are denoted as $\mathbf{r}_1$ and $\mathbf{r}_2$, and $q \equiv |\mathbf{r}_1 - \mathbf{r}_2|$. With the exception of the terms which give rise to H_{I3} and H_{I4} below, the additional terms in $U^{(1)}$ beyond the Fermi-Breit interaction do not contribute to the Zeeman effect (to order α^3). These terms are used and described in Sec. V.

In a previous paper [15] one of us (K.J.S.) has shown that the interaction of an arbitrary composite system with an external electromagnetic field can be written as the sum of two terms:

$$H_I = H_{I1} + H_{I2} . \qquad (3)$$

Here H_{I1} is the interaction resulting from a minimal substitution in the total Hamiltonian of the isolated composite system:

$$H_{I1} = i \sum_{\mu=1}^{2} \frac{e_\mu}{2c} \{ [\mathbf{r}_\mu, H] \cdot \mathbf{A}_\mu + \mathbf{A}_\mu \cdot [\mathbf{r}_\mu, H] \}$$

$$- \frac{1}{4c^2} \sum_{\mu=1}^{2} \sum_{\nu=1}^{2} \sum_{k=1}^{3} \sum_{j=1}^{3} e_\mu e_\nu \{ [r_{\mu,k}, [r_{\nu,j}, H]] A_{\mu,k} A_{\nu,j} + A_{\mu,k} A_{\nu,j} [r_{\mu,k}, [r_{\nu,j,H}]] \} , \qquad (4)$$

where e_μ and $\mathbf{r}_\mu$ are the charge and constituent position vector of particle μ, respectively, the vector potential $\mathbf{A}_\mu$ is taken as $\frac{1}{2}\mathbf{B} \times \mathbf{r}_\mu$ for the case of a constant external magnetic field, and we set $\hbar = 1$ throughout this paper. The second term H_{I2} includes the sum of spin-dependent terms resulting from the Foldy-Wouthuysen reduction of single Dirac particles with anomalous magnetic moments in an external electromagnetic field. For the case of a constant external magnetic field and no electric field we have

$$H_{I2} = - \sum_{\mu=1}^{2} \frac{e_\mu}{m_\mu c}(1+a_\mu)\mathbf{s}_\mu \cdot \mathbf{B}_\mu + \sum_{\mu=1}^{2} \frac{e_\mu}{4m_\mu^3 c^3}[p_\mu^2, \mathbf{s}_\mu \cdot \mathbf{B}_\mu]_+$$

$$- \sum_{\mu=1}^{2} \frac{e_\mu^2}{4m_\mu^3 c^4} \{ (\mathbf{A}_\mu \cdot \mathbf{p}_\mu + \mathbf{p}_\mu \cdot \mathbf{A}_\mu)\mathbf{s}_\mu \cdot \mathbf{B}_\mu + \text{H.c.} \}$$

$$- \sum_{\mu=1}^{2} \frac{e_\mu^2}{2m_\mu^3 c^4}(\mathbf{s}_\mu \cdot \mathbf{B}_\mu)^2 + \sum_{\mu=1}^{2} \frac{a_\mu e_\mu}{2m_\mu^3 c^3}(\mathbf{s}_\mu \cdot \mathbf{p}_\mu)(\mathbf{p}_\mu \cdot \mathbf{B}_\mu) , \qquad (5)$$

where p_μ, s_μ, m_μ, and a_μ are the momenta, spins, masses, and anomalous magnetic moment parameters of the constituent particles, respectively.

The above Hamiltonians [Eqs. (4) and (5)] contain terms which are both linear and quadratic in the external magnetic field. The lowest-order quadratic contributions that come from H_{I1} are used in Sec. V below and are found to be small although not completely negligible for the precision of the analysis presented here. The quadratic terms of H_{I2} are seen to be of order α^2 relative to the lowest-order quadratic terms in H_{I1} and are completely negligible.

For hydrogenlike atoms, if we set $e_1 = -e$, $e_2 = Ze$, $s_1 = \sigma_e/2$, $s_2 = \sigma_N/2$, $r_1 = r_e$, $r_2 = r_N$, $q = r_e - r_N$, $a_1 = a_e$, $a_2 = a_N$, $m_1 = m_e$, $m_2 = m_N$, $p_1 = p_e$, and $p_2 = p_N$ in Eqs. (1), (4), and (5) we can write

$$H + H_I = \sum_{n=0}^{7} H_n , \tag{6}$$

$$H_0 = \frac{\Pi_e^2}{2m_e} + \frac{\Pi_N^2}{2m_N} - \frac{Ze^2}{q} , \tag{7}$$

$$H_1 = -\frac{\Pi_e^4}{8m_e c^2} - \frac{\Pi_N^4}{8m_N c^2} , \tag{8}$$

$$H_2 = \frac{\pi Ze^2}{2m_e^2 c^2}(1 + 2a_e)\delta^3(q) - \frac{\pi Ze^2}{2m_N^2 c^2}(1 + 2a_N)\delta^3(q) , \tag{9}$$

$$H_3 = \frac{Ze^2}{4m_e^2 c^2}(1 + 2a_e)\sigma_e \cdot \frac{q \times \Pi_e}{q^3}$$
$$- \frac{Ze^2}{4m_N^2 c^2}(1 + 2a_N)\sigma_N \cdot \frac{q \times \Pi_N}{q^3} , \tag{10}$$

$$H_4 = -\frac{Ze^2}{2m_e m_N c^2}(1 + a_e)\sigma_e \cdot \frac{q \times \Pi_N}{q^3}$$
$$+ \frac{Ze^2}{2m_e m_N c^2}(1 + a_N)\sigma_N \cdot \frac{q \times \Pi_e}{q^3} , \tag{11}$$

$$H_5 = \frac{e}{2m_e c}\left[\sigma_e \cdot B\left(1 - \frac{\Pi_e^2}{2m_e}\right) \right.$$
$$\left. + a_e\left[\sigma_e \cdot B - \frac{(\sigma_e \cdot \Pi_e)(\Pi_e \cdot B)}{2m_e^2} \right] \right]$$
$$- \frac{Ze}{2m_N c}\left[\sigma_N \cdot B\left(1 - \frac{\Pi_N^2}{2m_N}\right) \right.$$
$$\left. + a_N\left[\sigma_N \cdot B - \frac{(\sigma_N \cdot \Pi_N)(\Pi_N \cdot B)}{2m_N^2} \right] \right] , \tag{12}$$

$$H_6 = \frac{Ze^2}{2m_e m_N c^2}\left[\frac{1}{q}(\Pi_e \cdot \Pi_N) + q\left(\frac{q}{q^3} \cdot \Pi_e\right) \cdot \Pi_N \right] , \tag{13}$$

$$H_7 = \frac{Ze^2}{4m_e m_N c^2}(1 + a_e)(1 + a_N)$$
$$\times \left[\frac{8\pi}{3}(\sigma_e \cdot \sigma_N)\delta^3(q) \right.$$
$$\left. + \frac{3(\sigma_e \cdot q)(\sigma_N \cdot q) - (\sigma_e \cdot \sigma_N)q^2}{q^5} \right] , \tag{14}$$

where σ_e and σ_N are Pauli matrices and

$$\Pi_e = p_e + \frac{e}{2c}B \times r_e , \quad \Pi_N = p_N - \frac{Ze}{2c}B \times r_N . \tag{15}$$

The equality expressed in Eq. (6) is correct up to but not including terms of the order $\alpha^2(\mu_B)^2$. We have expressed $H + H_I$ through Eqs. (6)–(15) in order to clearly show the relationship between the results which we will obtain in this paper and the results of Refs. [9–12]. Equations (6)–(14) are exactly the same as Eq. (40) of Grotch and Hegstrom [10]. The mechanical momenta (Π_e and Π_N) are quite different. Grotch and Hegstrom [10] would have mechanical momenta given by our Eq. (15) had they not made their unitary transformation [Eqs. (24)–(27) of Ref. [10]] and kept their Hamiltonian expressed in terms of the constituent variables. That is to say that Eqs. (6)–(15) above are equivalent to the Chraplyvy-Barker-Glover [10] reduction of the extended Breit equation expressed in terms of the constituent variables. This is clear from Ref. [10]. We would like to make it clear that our starting point is the same as that of Grotch and Hegstrom [10] and also of Refs. [9], [11], and [12]. We will take Eqs. (6)–(15) as our starting point. Grotch and Hegstrom would have obtained the same results [Eqs. (40) and (41) of Ref. [10]] if they had made their unitary transformation after the Chraplyvy-Barker-Glover reduction of the extended Breit equation expressed in terms of the constituent variables.

There are additional radiative and recoil corrections which must be added to H_I. Systematic and comprehensive analyses of the radiative effects of bound particles have been given by Erickson and Yennie [23] and Brodsky and Erickson [24]. It is well known and has been shown elsewhere [10] that there is no lowest-order energy shift due to vacuum polarization in a constant external magnetic field. Therefore, in lowest order we only need to consider the self-energy of the bound electron and recoil corrections. Following Brodsky and Erickson [24] we can decompose the lowest-order self-energy of a bound particle of mass m charge e and in state $|n\rangle$ into the sum of three parts:

$$\Delta E_n = \Delta E_n(L) + \Delta E_n(M) + \Delta E_n(R) , \tag{16}$$

where

$$\Delta E_n(L) = \frac{-2\alpha}{3\pi m^2 c^2}\left\langle n \left| \Pi_\mu \left[\ln\frac{m}{2(H - E_n)} \right. \right. \right.$$
$$\left. \left. \left. + \frac{11}{24} \right]\gamma_0[\Pi^\mu, H] \right| n \right\rangle , \tag{17}$$

$$\Delta E_n(M) = \frac{\alpha}{2\pi} \left[\frac{e}{2mc^2} \right] \langle n | \tfrac{1}{2}\sigma_{\mu\nu}F^{\mu\nu} | n \rangle , \tag{18}$$

and $\Delta E_n(R)$ contains terms quadratic in $F^{\mu\nu}$ (the electromagnetic-field tensor) and terms which modify the operators in Eqs. (17) and (18) at small distances. The terms in $\Delta E_n(R)$ do not contribute any terms of order α^3 or larger to the Zeeman shifts [24]. Above, $H - E_n = (1/2m)(m^2 - \Pi^2)$, $\Pi^\mu = p^\mu - eA^\mu$, and $\Pi = \gamma^\mu\Pi_\mu$. The Pauli interaction $\Delta E_n(M)$ accounts for the lowest-order contributions to the anomalous magnetic moment of the bound particle. In addition to $\Delta E_n(M)$ we must also include the contributions from $\Delta E_n(L)$ as first recognized by Grotch and Kashuba [9]. For the case of an electron of charge e Grotch and Kashuba have shown that $\Delta E_n(L)$ yields the following contribution to the Zeeman interaction [9]:

$$H_{I3} = \frac{\alpha e i}{3m_e^2 c^2} \int_0^\infty \frac{dk}{1 + 2k/m_e c^2}$$
$$\times \mathbf{B} \cdot \sum_{n'} \frac{\langle n | \mathbf{p}_e | n' \rangle \times \langle n' | \mathbf{p}_e | n \rangle}{k + \Delta E_{n'n}} , \tag{19}$$

where $\Delta E_{n'n}$ is the nonrelativistic energy difference $E_{n'} - E_n$ of the unperturbed bound states. This contribution must be evaluated numerically for any given state $| n \rangle$ and has not been included in any of the previous work. The analogous term coming from the self-energy of the proton is of order $(m_e/m_N)^3$ relative to H_{I3} and is completely negligible.

It is well known that the Fermi-Breit interaction accounts for single-photon exchange only approximately in the sense that in a nonrelativistic perturbative approach it neglects recoil in the intermediate states [25]. Therefore, in addition to the terms resulting from a minimal substitution in the Fermi-Breit interaction implicit in H_{I1} we must include recoil corrections to single-phonon exchange in the presence of a constant external magnetic field. Salpeter [25] evaluated all the $\alpha(Z\alpha)^4$ m_e/m_N recoil corrections to the Fermi-Breit interaction. It is clear from the latter work that to lowest order, $\alpha(Z\alpha)^2(m_e/m_N)^q$ ($q = 1, 2, \ldots, \infty$), we only need to consider the exchange of a single transverse photon between the electron and the nucleus in a constant external magnetic field using nonrelativistic perturbation theory. This is easily achieved by making a minimal substitution in Eq. (45) of Ref. [25]. The derivation of this term is presented in the Appendix and the result is

$$H_{I4} = \frac{2\alpha e i (m_e - m_N)}{3M^2 \mu^2 c^2}$$
$$\times \int_0^{\alpha m_e} dk \, \mathbf{B} \cdot \sum_{n'} \frac{\langle n | \mathbf{p}_e | n' \rangle \times \langle n' | \mathbf{p}_N | n \rangle}{k + \Delta E_{n'n}} , \tag{20}$$

where $M = m_e + m_N$ and $\mu = m_e m_N / M$.

Now we use the relativistic (to order $1/c^2$) relations of Krajcik and Foldy [21] to express the Hamiltonian $H + H_I = H + H_{I1} + H_{I2} + H_{I3} + H_{I4}$ in terms of the center of mass and internal variables. The Krajcik-Foldy relations are [21]

$$\mathbf{r}_\mu = \rho_\mu + \mathbf{R} - \frac{1}{2c^2} \left[\frac{\rho_\mu \cdot \mathbf{P}}{M} \left[\frac{\pi_\mu}{m_\mu} + \frac{\mathbf{P}}{2M} \right] + \text{H.c.} \right] - \frac{1}{2c^2} \sum_v \left[\frac{\pi_v^2 \rho_v}{2m_v M} + \text{H.c.} \right] + \sum_v \frac{(\rho_v \times \pi_v)}{2M^2 c^2} \times \mathbf{P}$$

$$- \frac{\Sigma_\mu \times \mathbf{P}}{2m_\mu Mc^2} + \sum_v \frac{\Sigma_v \times \pi_v}{2m_v Mc^2} + \sum_v \frac{\Sigma_v \times \mathbf{P}}{2M^2 c^2} - \frac{1}{M} \mathbf{W}^{(1)} - \frac{i}{M} \left[\int_0^P d\mathbf{p} \cdot \mathbf{W}^{(1)}, \rho_\mu \right] , \tag{21}$$

$$\mathbf{p}_\mu = \pi_\mu + \frac{m_\mu}{M} \mathbf{P} + \left[\frac{\pi_\mu^2}{2m_\mu} - \frac{m_\mu}{M} \sum_v \frac{\pi_v^2}{2m_v} + \frac{\pi_\mu \cdot \mathbf{P}}{2M} \right] \frac{\mathbf{P}}{Mc^2} - \frac{i}{M} \left[\int_0^P d\mathbf{p} \cdot \mathbf{W}^{(1)}, \pi_\mu \right] , \tag{22}$$

$$\mathbf{s}_\mu = \Sigma_\mu - \frac{\Sigma_\mu \times (\pi_\mu \times \mathbf{P})}{2m_\mu Mc^2} - \frac{i}{M} \left[\int_0^P d\mathbf{p} \cdot \mathbf{W}^{(1)}, \Sigma_\mu \right] , \tag{23}$$

where $\mathbf{r}_\mu$, $\mathbf{p}_\mu$, and $\mathbf{s}_\mu$ are the constituent position, momenta, and spin variables, respectively, and ρ_μ, π_μ, and Σ_μ are the internal position, momenta, and spin variables. The position and momentum variables of the center of mass are denoted by $\mathbf{R}$ and $\mathbf{P}$. The interaction-dependent part of the Lorentz boost operator ($\mathbf{W}^{(1)}$) for the two-body case was found by Sebastian and Yun [16] to be

$$\mathbf{W}^{(1)} = \left[\frac{e_1 e_2}{2c^2} \right] \frac{\rho_1 + \rho_2}{|\rho_1 - \rho_2|} . \tag{24}$$

The matrix elements of the resulting interaction Hamiltonian contains factors of R and P. Matrix elements of R in states of definite momenta are ambiguous. Therefore, before we get to the $\mathbf{P} \rightarrow 0$ limit we must take the ex-

pectation values of these operators using a symmetric normalized wave packet:

$$\Psi = \frac{1}{(\pi\lambda)^{3/4}} e^{-R^2/2\lambda} , \tag{25}$$

which in the $\lambda \rightarrow \infty$ limit is equivalent to the $\mathbf{p} = 0$ plane wave. Once this is done we get an unambiguous operator $(H + H_I)$ in the $\mathbf{P} = 0$ frame. It is important to note that we can use this procedure because the use of the Krajcik-Foldy relations ensure that the generators of the Poincaré group (in particular the Hamiltonian and the Lorentz boost operator) can be written in their single particle form [21]. Consequently, the atomic wave functions of definite total momentum P can be written as the prod-

uct of a plane wave and the internal wave functions.

For the case of hydrogenlike atoms of nuclear spin I and electronic spin S_e we set $\Sigma_1 = S_e = \sigma_e/2$, $\Sigma_2 = I = \sigma_N/2$, $\pi_1 = \pi$, $\pi_2 = -\pi$, $\rho_1 = (m_N/M)q$, and $\rho_2 = -(m_e/M)q$, where $q = \rho_e - \rho_N$. Equations (6)–(14) retain their same form and now Eq. (15) becomes

$$\Pi_e = \pi + \frac{e}{2c}B \times \left\{ \frac{m_N}{m_e}q - \frac{1}{4M^2c^2}\left[\pi^2 q \left[\frac{m_N}{m_e} - \frac{m_e}{M_N} \right] \right. \right.$$

$$+ \text{H.c.} \Big]$$

$$+ \frac{1}{2Mm_ec^2}\left[S_e - \frac{m_e}{m_N}I \right] \times \pi$$

$$+ \frac{Ze^2}{2M^2c^2}(m_N - m_e)\frac{q}{q} \Big\}, \qquad (26)$$

$$\Pi_p = -\pi - \frac{Ze}{2c}B \times \left\{ \frac{-m_e}{m_N}q - \frac{1}{4M^2c^2}\left[\pi^2 q \left[\frac{m_N}{m_e} - \frac{m_e}{m_N} \right] \right. \right.$$

$$+ \text{H.c.} \Big]$$

$$+ \frac{1}{2Mm_ec^2}\left[S_e - \frac{m_e}{m_N}I \right] \times \pi$$

$$+ \frac{Ze^2}{2M^2c^2}(m_N - m_e)\frac{q}{q} \Big\}. \qquad (27)$$

After some algebra the linear Zeeman Hamiltonian can be extracted from Eqs. (6)–(14), (26), (27), (19), and (20). Choosing the z axis along the direction of the magnetic field, we obtain

$$H_I^L = \eta_L BL_z + \eta_S BS_{ez} + \eta_I BI_z + \eta_q Bq_z + \eta_\pi B\pi_z + \chi_z B, \qquad (28)$$

$$\eta_L = \frac{e}{2m_ec}\left\{ 1 - \frac{Zm_e}{m_N} + (Z-1)\frac{m_e}{M} \right.$$

$$\left. - \frac{\pi^2}{2M^2c^2}\left[\left[\frac{m_N}{m_e} - \frac{m_e}{m_N} \right] \left[1 - Z\frac{m_e}{m_N} \right] + M\left[\frac{m_N}{m_e^2} - Z\frac{m_e^2}{m_N^3} \right] \right] - \frac{Ze^2}{2c^2}\frac{1}{q}\left[\frac{2(1-Z)m_e}{M^2} \right] \right\}, \qquad (29)$$

$$\eta_S = \frac{e}{m_ec}\left\{ 1 + a_e - \frac{\pi^2}{4c^2}\left[\frac{2}{m_e^2} + \frac{Z}{m_NM} + \frac{1}{m_eM} \right] + \frac{Ze^2}{4qc^2}\left[\frac{(1+2a_e)}{m_e} - \frac{2Z(1+a_e)}{m_N} + \frac{1}{M}[2Z - 1 + 2(Z-1)a_e] \right] \right\}, \qquad (30)$$

$$\eta_I = \frac{-Ze}{m_Nc}\left\{ 1 + a_N - \frac{\pi^2}{4Zc^2}\left[\frac{2Z}{m_N^2} + \frac{Z}{m_NM} + \frac{1}{m_eM} \right] + \frac{e^2}{4qc^2}\left[\frac{Z(1+2a_N)}{m_N} - \frac{2(1+a_N)}{m_e} + \frac{1}{M}[2 - Z + 2(1-Z)a_N] \right] \right\}, \qquad (31)$$

$$\eta_q = \frac{e}{m_ec}\left\{ \frac{-Ze^2}{4c^2}\frac{1}{q^3}(S_e \cdot q)\left[\frac{(1+2a_e)}{m_e} - \frac{2Z(1+a_e)}{m_N} + \frac{1}{M}[2Z - 1 + 2(Z-1)a_e] \right] \right.$$

$$\left. + \frac{Ze^2}{4c^2}\frac{1}{q^3}(I \cdot q)\left[\frac{m_e}{m_N} \right]\left[\frac{Z(1+2a_N)}{m_N} - \frac{2(1+a_N)}{m_e} + \frac{1}{M}[2 - Z + 2(1-Z)a_N] \right] \right\}, \qquad (32)$$

$$\eta_\pi = \frac{e}{m_ec}\left\{ \frac{1}{4c^2}(S_e \cdot \pi)\left[\frac{Z}{m_NM} + \frac{1}{m_eM} - \frac{2a_e}{m_e^2} \right] - \frac{1}{4c^2}(I \cdot \pi)\left[\frac{m_e}{m_N} \right]\left[\frac{Z}{m_NM} + \frac{1}{m_eM} - \frac{2Za_N}{m_N^2} \right] \right\}, \qquad (33)$$

$$\chi_z = \frac{\alpha ei}{4m_e^3c^2}\int_0^\infty \frac{dk}{1 + 2k/m_ec^2}\sum_{n'}\left[\frac{\langle n|\pi_x|n'\rangle\langle n'|\pi_y|n\rangle}{k + \Delta E_{n'n}} - \text{c.c.} \right]$$

$$+ \frac{2\alpha ei(m_e - m_N)}{3M^2\mu^2c^2}\int_0^{\alpha m_e}dk\sum_{n'}\left[\frac{\langle n|\pi_x|n'\rangle\langle n'|\pi_y|n\rangle}{k + \Delta E_{n'n}} - \text{c.c.} \right]. \qquad (34)$$

In Eqs. (28)–(34) $L = q \times \pi$. The evaluation of $H_{I3} + H_{I4} = \chi_z B$ is outlined in the Appendix. This interaction turns out to be proportional to L_z. This is to be expected since it must be proportional to the z component of a vector operator and it is a spin-independent interaction acting in the Lm_L subspace. Using these results we can write

$$H_{I3}+H_{I4}=B\chi_z=a(n,L,m_L)L_z \ , \tag{35a}$$

where

$$a(n,L,-m_L)=-a(n,L,m_L) \tag{35b}$$

and the coefficients are

$$a(2,1,1)=2.3203\times10^{-7} \text{ MHz/G} \ ,$$

$$a(3,1,1)=5.5292\times10^{-9} \text{ MHz/G} \ ,$$

$$a(3,2,1)=1.9964\times10^{-9} \text{ MHz/G} \ , \tag{35c}$$

$$a(3,2,2)=1.9965\times10^{-9} \text{ MHz/G} \ ,$$

for hydrogen. Positronium has no orbital magnetic moment and χ_z vanishes in this case.

For neutral systems Eqs. (28)–(33) (neglecting the χ_z term) are in agreement with the interaction Hamiltonian of Grotch and Hegstrom [10] to order $\alpha(Z\alpha)^2$ and all orders in m_e/m_N. In fact, for neutral systems we can obtain Eqs. (6)–(14) with (26) and (27) [and consequently (28)–(33)] by making a unitary transformation of the Hamiltonian of Grotch and Hegstrom [10] [Eqs. (40) and (41) of Ref. [10]] with the following unitary operator:

$$U=\exp\left[\frac{ie}{4}(\mathbf{r}_e-\mathbf{r}_N)\cdot\mathbf{B}\times\left\{\frac{1}{4M^2c^2}\left[\pi^2\mathbf{q}\left(\frac{m_N}{m_e}-\frac{m_e}{m_N}\right)\right]+\text{H.c.}\right.\right.$$
$$\left.\left.+\frac{1}{Mm_ec^2}\left[\mathbf{S}_e-\frac{m_e}{m_N}\mathbf{I}\right]\times\pi+\frac{Ze^2}{2M^2c^2}(m_N-m_e)\frac{\mathbf{q}}{q}\right\}+\text{H.c.}\right] \ . \tag{36}$$

It is well known that two Hamiltonians which are unitarily equivalent have the same energy eigenvalues. Thus, as we shall see below, for neutral systems, we obtain the same results as Grotch and Kashuba [9] for the g_J and g_I factors of hydrogenlike atoms of nuclear spin $\frac{1}{2}$ and we obtain the same results as Lewis and Hughes [12] for the energy eigenvalues of positronium.

The results of Grotch and Kashuba [9] and of Grotch and Hegstrom [10] are strictly only correct for neutral systems or for $Z=1$. For charged systems Grotch and co-workers point out that there are additional "small corrections" to their results [10]. This is true because the unitary transformation which they use to eliminate the center-of-mass dependence of the Hamiltonian is only correct for neutral systems. The additional terms that are introduced for $Z\neq1$ in our linear Zeeman Hamiltonian [Eqs. (28)–(34)] beyond those in the aforementioned work are as large as $(Z\alpha)^2m_{e/m_N}$ and $\alpha(Z\alpha)^2m_e/m_N$ and are found in η_L, η_s, η_I, and η_q [compare with Eq. (43) of Ref. [10] and Eq. (1) of Ref. [9]]. However, when the expectation values of the π^2 and $1/q$ operators are taken using the reduced mass, fortuitous algebraic cancellations eliminate the contribution of these terms to the g factors such that the g factors obtained here agree with those obtained by Grotch and Kashuba [9] to at least order $\alpha(Z\alpha)^2m_e/m_N$ for all atoms. This seems to support the claim of Ref. [10] that the effect of these additional terms for hydrogenlike ions are small [10].

Setting $m_N=m_e$ and $a_N=a_e$ in Eqs. (28)–(33) we can write the linear Zeeman Hamiltonian for positronium as

$$H_p=\frac{eB}{m_ec}\left\{\left[(1+a_e)-\frac{e^2}{8m_ec^2}\frac{1}{q}-\frac{3}{4}\frac{\pi^2}{m_e^2c^2}\right](S_{ez}-I_z)\right.$$

$$+\frac{e^2}{8m_ec^2}\frac{1}{q^3}[(\mathbf{S}_e-\mathbf{I})\cdot\mathbf{q}q_z]$$

$$\left.-\frac{1}{4m_e^2c^2}(2a_e-1)[(\mathbf{S}_e-\mathbf{I})\cdot\pi\pi_z]\right\} \ . \tag{37}$$

We can obtain Eq. (37) from the positronium Hamiltoni-

an of Grotch and Kashuba [9] and of Lewis and Hughes [12] with the unitary operator of Eq. (36) with $m_e=m_N$.

III. THE g_I AND g_J FACTORS

Taking the same approach as Grotch and Kashuba [9] we can use the projection theorem to define the g_I and g_J factors in the $|nFm_FJL\rangle$ representation:

$$\langle nFm_FJL|H_I^L|nFm_FJL\rangle$$

$$=\left\langle nFm_FJL\left|\left[\frac{e}{2m_ec}g_J\mathbf{J}-\frac{Ze}{2m_Nc}g_I\mathbf{I}\right]\cdot\mathbf{B}\right|nFm_FJL\right\rangle \ , \tag{38}$$

where $\mathbf{J}=\mathbf{S}_e+\mathbf{L}$ is the total electronic angular momentum and $\mathbf{F}=\mathbf{J}+\mathbf{I}$ is the total angular momentum of the atom. The g_J and g_I factors will be independent of m_F. Therefore, we may evaluate Eq. (38) with $m_F=F$. Expanding Eq. (38) for the g_I factor we can write

$$\frac{-Ze}{2m_Nc}\frac{F(F+1)+I(I+1)-J(J+1)}{2(F+1)}g_I$$

$$=\langle nFFJL|\eta_II_z+\eta_q'q_z+\eta_\pi'\pi_z|nFFJL\rangle \ , \tag{39}$$

where η_q' consists of only those terms in η_q [Eq. (32)] which contain the $(\mathbf{I}\cdot\mathbf{q})$ factor and η_π' consists of only those terms in η_π [Eq. (33)] which contain the $(\mathbf{I}\cdot\pi)$ factor. The terms in H_I^L which contribute to g_J act only in a (J,m_J) representation and g_J can be evaluated in this representation such that

$$\frac{e}{2m_ec}g_JJ=\langle nJJLS_e|\eta_LL_z+\eta_sS_{eZ}+\eta_q''q_z$$

$$+\eta_\pi''\pi_Z+a(n,L,m_L)L_Z|nJJLS_e\rangle \ , \tag{40}$$

where η_q'' consists of only those terms in η_q [Eq. (32)] which contain the $(\mathbf{S}_e\cdot\mathbf{q})$ factor and η_π'' consists of only those terms in η_π [Eq. (33)] which contain the $(\mathbf{S}_e\cdot\pi)$ factor.

Since m_L is not a good quantum number in the

$|nJm_JLS_e\rangle$ representation the $a(n,L,m_L)L_z$ terms in Eq. (38) require special treatment. Setting $S=S_e$ we write the expansion

$$|Jm_JLS\rangle = \sum_{m_L}\sum_{m_s}|Lm_LSm_s\rangle\langle Lm_LSm_s;Jm_J\rangle \ . \qquad (41)$$

We can express these contributions to the g_J factor as

$$g_J' = \frac{1}{\mu_B J}\sum_{m_L}\sum_{m_{s_e}}|\langle JJ;Lm_LS_e m_{s_e}\rangle|^2 m_L\, a(n,L,m_L) \ , \qquad (42)$$

where μ_B is the Bohr magneton. The $a(n,L,m_L)$ coefficients were given by Eqs. (35b) and (35c). The matrix elements of other operators which act only in either the (I,m_I) space or the (J,m_J) space can easily be evaluated to get

$$\langle nJJLS_e|L_Z|nJJLS_e\rangle$$
$$= \frac{J(J+1)+L(L+1)-S_e(S_e+1)}{2(J+1)} \ ,$$

$$\langle nJJLS_e|S_z|nJJLS_e\rangle$$
$$= \frac{J(J+1)-L(L+1)+S_e(S_e+1)}{2(J+1)} \ , \qquad (43)$$

$$\left\langle nJJLS_e\left|\frac{(\mathbf{S}_e\cdot\mathbf{q})q_z}{q^3}\right|nJJLS_e\right\rangle$$

$$= \frac{\left\langle nJJLS_e\left|\frac{(\mathbf{S}_e\cdot\hat{\mathbf{q}})(\hat{\mathbf{q}}\cdot\mathbf{J})}{q}\right|nJJLS_e\right\rangle}{(J+1)} = \frac{c\mu Z\alpha/n^2}{4(J+1)} \ ;$$

$$\langle nJJLS_e|(\mathbf{S}_e\cdot\boldsymbol{\pi})\pi_z|nJJLS_e\rangle$$

$$= \frac{\langle nJJLS_e|(\mathbf{S}_e\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\mathbf{J})|nJJLS_e\rangle}{(J+1)} = \frac{(c\mu Z\alpha/n)^2}{4(J+1)} \ , \qquad (44)$$

$$\langle nFFJL|I_z|nFFJL\rangle = \frac{F(F+1)+I(I+1)-J(J+1)}{2(F+1)} \ ,$$

where use is made the fact that

$$\langle\pi^2\rangle = (c\mu Z\alpha/n)^2 \ , \quad \left\langle\frac{1}{q}\right\rangle = c\mu Z\alpha/n^2 \ . \qquad (45)$$

We also have

$$\left\langle nFFJL\left|\frac{(\mathbf{I}\cdot\mathbf{q})q_z}{q^3}\right|nFFJL\right\rangle$$

$$= \left\langle nFFJL\left|\frac{(\mathbf{I}\cdot\hat{\mathbf{q}})(\hat{\mathbf{q}}\cdot\mathbf{F})}{(F+1)q}\right|nFFJL\right\rangle \qquad (46)$$

and

$$\left\langle nFFJL|(\mathbf{I}\cdot\boldsymbol{\pi})\pi_z|nFFJL\right\rangle$$

$$= \left\langle nFFJL\left|\frac{(\mathbf{I}\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\mathbf{F})}{(F+1)}\right|nFFJL\right\rangle \ .$$

The matrix elements of $(\mathbf{I}\cdot\hat{\mathbf{q}})$ implicit in Eq. (46) do not have explicit expressions for arbitrary I. Therefore, we must choose a specific value for the nuclear spin. For nuclear spin $\frac{1}{2}$, $(\mathbf{I}\cdot\hat{\mathbf{q}})(\hat{\mathbf{q}}\cdot\mathbf{F}) = \frac{1}{4}+(\mathbf{I}\cdot\hat{\mathbf{q}})(\hat{\mathbf{q}}\cdot\mathbf{S}_e)$ and $(\mathbf{I}\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\mathbf{F}) = \pi^2/4+(\mathbf{I}\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\mathbf{S}_e)$. The last two terms in these expressions are scalar products of vector operators which act in separate spaces $[(Jm_J),(I,m_I)]$. Using $6j$ symbols they can be evaluated to get

$$\left\langle nFFJL\left|\frac{(\mathbf{I}\cdot\hat{\mathbf{q}})(\hat{\mathbf{q}}\cdot\mathbf{F})}{(F+1)q}\right|nFFJL\right\rangle$$

$$= \frac{\mu Z\alpha c/n^2}{4(F+1)} + (-1)^{J+I+F}\begin{Bmatrix}J & I & F\\ I & J & 1\end{Bmatrix}\langle J\|s\|J\rangle$$

$$\times\langle I\|I\|I\rangle\frac{1}{(F+1)} \ ,$$

$$\left\langle nFFJL\left|\frac{(\mathbf{I}\cdot\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\mathbf{F})}{(F+1)}\right|nFFJL\right\rangle \qquad (47)$$

$$= \frac{(\mu Z\alpha c/n)^2}{4(F+1)} + (-1)^{J+I+F}\begin{Bmatrix}J & I & F\\ I & J & 1\end{Bmatrix}$$

$$\times\langle J\|s'\|J\rangle\langle I\|I\|I\rangle\frac{1}{(F+1)} \ ,$$

where $\langle J\|s\|J\rangle$, $\langle I\|I\|I\rangle$ and $\langle J\|s'\|J\rangle$ are reduced matrix elements obtained from $\hat{\mathbf{q}}(\mathbf{S}_e\cdot\hat{\mathbf{q}})/q$, $\mathbf{I}$, and $\boldsymbol{\pi}(\mathbf{S}_e\cdot\boldsymbol{\pi})$, respectively. The reduced matrix elements are found to be

$$\langle J\|s\|J\rangle = \frac{\mu Z\alpha c/n^2}{4}(2J+1)^{1/2}[J(J+1)]^{-1/2} \ ,$$

$$\langle J\|s'\|J\rangle = \frac{(\mu Z\alpha c/n)^2}{4}(2J+1)^{1/2}[J(J+1)]^{-1/2} \ , \qquad (48)$$

$$\langle I\|I\|I\rangle = [(2I+1)I(I+1)]^{1/2} \ .$$

The $6j$ symbols can be found in Ref. [26].

Using Eqs. (38), (39), (32), (42), (43), (47), and (48) the linear Zeeman Hamiltonian for hydrogenlike atoms of nuclear spin $\frac{1}{2}$ can be written as

$$H_I^L = \left\{\frac{e}{2m_e c}g_J\left[\frac{F(F+1)+J(J+1)-I(I+1)}{2F(F+1)}\right]\right.$$

$$\left.-\frac{Ze}{2m_N c}g_I\left[\frac{F(F+1)-J(J+1)+I(I+1)}{2F(F+1)}\right]\right\}$$

$$\times\mathbf{F}\cdot\mathbf{B} \ , \qquad (49)$$

with g_J and g_I given by

$$g_J = \frac{J(J+1)+L(L+1)-S_e(S_e+1)}{2J(J+1)} \left\{ 1 - \frac{Zm_e}{m_N} + (Z-1)\frac{m_e}{m_N} + \frac{\mu\varepsilon}{M^2} \left[\left[\frac{m_N}{m_e} - \frac{m_e}{m_N} \right] \left[1 - Z\frac{m_e}{m_N} \right] \right. \right.$$

$$\left. \left. + M\left[\frac{m_N}{m_e^2} - Z\frac{m_e^2}{m_N^3} \right] \right] + \varepsilon\left[\frac{2(1-Z)m_e}{M^2} \right] \right\}$$

$$+ \frac{J(J+1)-L(L+1)+S_e(S_e+1)}{J(J+1)} \left\{ 1 + a_e + \frac{\mu\varepsilon}{2}\left[\frac{2}{m_e^2} + \frac{Z}{m_N M} + \frac{1}{m_e M} \right] \right.$$

$$\left. - \frac{\varepsilon}{2}\left[\frac{(1+2a_e)}{m_e} - \frac{2Z(1+a_e)}{m_N} + \frac{1}{M}[2Z-1+2(Z-1)a_e] \right] \right\}$$

$$+ \frac{\varepsilon}{4J(J+1)} \left\{ \left[\frac{(1+2a_e)}{m_e} - \frac{2Z(1+a_e)}{m_N} + \frac{1}{M}[2Z-1+2(Z-1)a_e] \right] - \mu\left[\frac{Z}{m_N M} + \frac{1}{m_e M} - \frac{2a_e}{m_e^2} \right] \right\} + g_J' , \qquad (50)$$

$$g_I = 2(1+a_N) + \frac{\varepsilon\mu}{Z}\left[\frac{2Z}{m_N^2} + \frac{Z}{m_N M} + \frac{1}{m_e M} \right] - \frac{\varepsilon}{2}\left[\frac{Z(1+2a_N)}{m_N} - \frac{2(1+a_N)}{m_e} + \frac{1}{M}[2-Z+2(1-Z)a_N] \right]$$

$$+ \frac{\varepsilon}{4J(J+1)Z}\left[\frac{F(F+1)+J(J+1)-I(I+1)}{F(F+1)+I(I+1)-J(J+1)} \right]$$

$$\times \left\{ \left[\frac{Z(1+2a_N)}{m_N} - \frac{2(1+a_N)}{m_e} + \frac{1}{M}[2-Z+2(1-Z)a_N] \right] - \mu\left[\frac{Z}{m_N M} + \frac{1}{m_e M} - \frac{2Za_N}{m_N^2} \right] \right\} , \qquad (51)$$

where $\varepsilon = -\mu/2(Z\alpha/n)^2$ is the nonrelativistic binding energy. To be consistent to order α^3 we must use $a_e = \alpha/2\pi$ for the value of the anomalous magnetic moment parameter in the relativistic part of the interaction Hamiltonian and $a_e = \alpha/2\pi - 0.328\,478\,965(\alpha/\pi)^2 + 1.176\,11(\alpha/\pi)^3$ for the corresponding value in the non-relativistic part. This last value for a_e (to order α^3) is the latest CODATA [27] recommended value. The most recent CODATA recommended values for the fundamental constants were used for all of the numerical calculations of this paper [28] including the calculation of the results of other work for comparison. We have no other choice than to use the experimental value for the nuclear anomalous magnetic moment parameter. The above g factors for hydrogenlike atoms of atomic number Z and nuclear spin $\frac{1}{2}$ are correct to order $\alpha(Z\alpha)^2$ and all orders in m_e/m_N. The results of Grotch and Kashuba [9] are verified after expanding the above g factors in terms of the small parameters m_e/m_N, ε/m_e, ε/m_N, a_e, and a_N and keeping terms only of the first order in m_e/m_N.

In Table I the numerical values for the g_J and g_I factors for all of the $n=1$, 2, and 3 states of hydrogen using Eqs. (50) and (51) above are compared with the expressions for the g factors to order $\alpha^3 m_e/m_N$ given by Grotch and Kashuba [9]. Excluding the effect of g_J' the results presented here are in agreement with the work of Grotch and Kashuba [9] to within one part in 10^{11}–10^{12}. This is to be expected since Grotch and Kashuba have expanded their g factors to terms of order $\alpha^3 m_e/m_N \approx 10^{-11}$ and our g factors are correct to all orders in m_e/m_N. The effect of g_J' is small and is seen to manifest itself at the 10^{-7} and 10^{-9} levels for the $L \neq 0$

$n=2$ and 3 states, respectively.

There are two experimental quantities which are of principal interest. These are the ratio of the electronic to nuclear g factors for the ground state of hydrogen and the ratio of the electronic g factor of the $1S$ state of hydrogen to that of the $1S$ state of deuterium. These quantities are listed in Table II and are compared with previous works. All the results presented in Table II are in excellent agreement with the results of Hughes and Robinson [29], who experimentally determined the hydrogen-deuterium g-factor ratio to be $1+(7.2\pm1.2)\times10^{-9}$. They are in slight disagreement with the results of Larson, Valberg, and Ramsey [30], who obtained $1+(9.4\pm1.4)\times10^{-9}$. The electron-proton g factor ratio in Table II can be used as a theoretical correction to the measured value of $g_J m_N/g_I m_e$. Moreover Winkler et al. [31] have measured this to be $658.210\,706(6)$. We are in excellent agreement with this result and obtain $g_J m_N/g_I m_e = 658.210\,710$.

IV. THE POSITRONIUM g FACTOR

The Zeeman Hamiltonian for positronium [Eq. (37)] is a function of the difference between the spins of the electron and of the positron. The representation chosen for positronium is usually the $|Fm_F LS\rangle$ representation, where S is the total spin angular momentum and $\mathbf{F} = \mathbf{L} + \mathbf{S}$ is the total angular momentum. In this representation the total Hamiltonian (nonrelativistic and relativistic corrections and the linear Zeeman Hamiltonian) is diagonal in m_F which is a "good" quantum number.

TABLE I. The g_J and g_I factors for hydrogen. The first row of each entry is the result of this work. The second row of each entry is the result of Ref. [9].

State	g_J	g_I	$10^7 g_J'$
$1S_{1/2}$ $F=0$	2.002 283 852 451	5.585 546 196 562	
	2.002 283 852 483	5.585 546 196 659	
$1S_{1/2}$ $F=1$	2.002 283 852 451	5.585 595 721 693	
	2.002 283 852 483	5.585 595 721 773	
$2S_{1/2}$ $F=0$	2.002 310 440 943	5.585 657 628 141	
	2.002 310 440 951	5.585 657 628 165	
$2S_{1/2}$ $F=1$	2.002 310 440 943	5.585 670 009 423	
	2.002 310 440 951	5.585 650 009 443	
$2P_{1/2}$ $F=0$	0.665 158 751 846	5.585 657 628 140	2.210 40
	0.665 158 530 813	5.585 657 628 164	
$2P_{1/2}$ $F=1$	0.665 158 751 846	5.585 670 009 423	2.210 40
	0.665 158 530 813	5.585 650 009 443	
$2P_{3/2}$ $F=1$	1.333 736 376 777	5.585 645 246 858	1.105 20
	1.333 736 266 263	5.585 645 246 886	
$2P_{3/2}$ $F=2$	1.333 736 376 777	5.585 665 056 910	1.105 20
	1.333 736 266 263	5.585 665 056 931	
$3S_{1/2}$ $F=0$	2.002 315 364 738	5.585 678 263 618	
	2.002 315 364 741	5.585 678 263 628	
$3S_{1/2}$ $F=1$	2.002 315 364 738	5.585 683 766 410	
	2.002 315 364 741	5.585 683 766 419	
$3P_{1/2}$ $F=0$	0.665 163 468 623	5.585 678 263 618	0.052 67
	0.665 163 463 358	5.585 678 263 628	
$3P_{1/2}$ $F=1$	0.665 163 468 623	5.585 683 766 410	0.052 67
	0.665 163 463 358	5.585 683 766 419	
$3P_{3/2}$ $F=1$	1.333 740 207 961	5.585 672 760 826	0.026 33
	1.333 740 205 331	5.585 672 760 838	
$3P_{3/2}$ $F=2$	1.333 740 207 961	5.585 681 565 293	0.026 33
	1.333 740 205 331	5.585 681 565 303	
$3D_{3/2}$ $F=1$	0.798 879 446 106	5.585 672 760 826	0.013 31
	0.798 879 444 777	5.585 672 760 838	
$3D_{3/2}$ $F=2$	0.798 879 446 106	5.585 681 565 293	0.013 31
	0.798 879 444 777	5.585 681 565 303	
$3D_{5/2}$ $F=2$	1.200 025 129 371	5.585 674 961 942	0.011 41
	1.200 025 128 232	5.585 674 961 954	
$3D_{5/2}$ $F=3$	1.200 025 129 371	5.585 657 628 140	0.011 41
	1.200 025 128 232	5.585 657 628 164	

The linear Zeeman Hamiltonian connects states with $\Delta S = \pm 1$, $\Delta L = 0, \pm 2$. Therefore, we can define a g factor for the ground state as

$$\langle 1\,^3S_1 m_F = 0 | H_p | 1\,^1S_0 m_F = 0 \rangle$$

$$= \mu_B g \langle 1\,^3S_1 m_F = 0 | (\mathbf{S}_e - \mathbf{I}) \cdot \mathbf{B} | 1\,^1S_0 m_F = 0 \rangle . \quad (52)$$

Using H_p of Eq. (37) we get the same results as Grotch and Kashuba [9] and Lewis and Hughes [12]:

TABLE II. g-factor ratios of experimental interest.

Author(s)	$\dfrac{g_J(H,1s)}{g_I(H,1s)}$	$\left[\dfrac{g_p}{g_e}\right]^{-1}$	$\dfrac{g_J(H,1s)}{g_J(D,1s)} - 1$
This work	2.7724×10^{-8}		7.2209×10^{-9}
Grotch and Kashuba[a]	2.7726×10^{-8}		7.2328×10^{-9}
Faustov[b]	2.7820×10^{-8}		7.2324×10^{-9}
Close and Osborn[c]	2.7791×10^{-8}		7.2211×10^{-9}

[a]Reference [9].
[b]Reference [13].
[c]Reference [14].

$$g = 2\left[1 + a_e - \frac{5\alpha^2}{24} - \frac{\alpha^2}{24} a_e\right] . \quad (53)$$

This g factor is needed by experimentalists to determine the hyperfine-structure separation in the ground state of positronium. The separation $v = {}^3S_1 - {}^1S_0$ is measured by inducing a transition between the $m_F = 0$ and ± 1 levels of orthopositronium. The frequency of this transition is given from degenerate perturbation theory as [9]

$$f = \tfrac{1}{2} v \{[1 + (4\mu_B^2 B^2 g^2 / v^2)]^{1/2} - 1\} . \quad (54)$$

The experimentalists determine v by measuring f and B and correcting for f due to annihilation [32]. The most recent experiments use the g factor of Eq. (53) to obtain a measured value of $v = 203.389\,10(74)$ GHz with one experimental standard deviation being 3.6 ppm of the determined value [32].

V. THE ZEEMAN SPLITTINGS

The nonrelativistic internal Hamiltonian $h^{(0)}$ and its first-order relativistic correction $h^{(1)}$ are given by

$$h^{(0)} \equiv \sum_{\mu=1}^{n} \frac{\pi_\mu^2}{2m_\mu} + U^{(0)} ,$$

$$h^{(1)} \equiv - \sum_{\mu=1}^{n} \frac{\pi_\mu^4}{8m_\mu^3 c^2} + U^{(1)} \Bigg|_{P=0} , \tag{55}$$

where $U^{(0)}$ is simply the Coulomb interactions between the constituent particles. We shall take $U^{(1)}$ to be primarily given by the well-known Fermi-Breit interaction [21,22]. The Fermi-Breit interaction includes all of the $(Z\alpha)^4$ contributions to the zero-field energy-level splittings and with the phenomenological introduction of the anomalous magnetic moments of the constituent particles it also includes some of the $\alpha(Z\alpha)^4$ contributions and even terms of order $\alpha^2(Z\alpha)^4$ coming from terms which contain the product of the two anomalous magnetic moment parameters. All the bound-state corrections of order α^6 have not been evaluated at this time and the $\alpha^2(Z\alpha)^4$ terms will not be retained. All of the $\alpha(Z\alpha)^4$ contributions for the $n=1$ and 2 levels of a two-body system have been computed by Fulton and Martin [33]. It is a simple matter to generalize their results for $n=3$ and add these corrections to the Fermi-Breit interaction with anomalous magnetic moments so that we are correct to order $\alpha(Z\alpha)^4$ inclusive for the first three levels of hydrogen and positronium. The results of Fulton and Martin, however, are not correct for $n\neq2$ S states [34]. The correct results can be obtained from Eq. (3.9) of Gupta, Repko, and Suchyta [34]. The numerical values of the corrections of order $\alpha(Z\alpha)^4$ which must be added to the Fermi-Breit interaction with anomalous magnetic moments are listed in Table III.

Furthermore, if a proper analysis of hydrogen in the $|nFm_FJL\rangle$ representation is to be presented we must account for the Lamb shift. Comprehensive analyses of the Lamb shift have been given by Erickson and Yennie [23] and Brodsky and Erickson [24]. The $\alpha(Z\alpha)^4$ contributions of Fulton and Martin [33] and Gupta, Repko, and Suchyta [34] contain some of the relativistic and recoil corrections to the Lamb shift. In addition there are vacuum polarization corrections, reduced mass corrections, higher-order radiative corrections, and finite nuclear charge distribution corrections [23]. Additionally, Bhatt and Grotch [35] have worked out the radiative recoil corrections of order $\alpha(Z\alpha)^5 m_e/m_N$. More recently Don-

cheski, Grotch, and Erickson [36] have calculated all the pure recoil corrections to order $(Z\alpha)^6 m_e/m_N$. All of these corrections to the zero-field splittings of hydrogen will be included to reflect the current knowledge of the hydrogen spectrum. The numerical corrections which must be added to the Fermi-Breit interaction with anomalous magnetic moments and $\alpha(Z\alpha)^4$ corrections of Table III are listed in Table IV. Finally, we must include the lowest-order annihilation interaction in the case of positronium:

$$U_A^{(1)} = \frac{\pi\alpha}{m_e^2 c^2} (S)^2 \delta^3(\mathbf{q}) . \tag{56}$$

The linear Zeeman Hamiltonians were presented in Eqs. (28)–(34) and (37). The lowest-order nonrelativistic quadratic Zeeman Hamiltonian for hydrogen (we will call it H_f^Q) can also be obtained from Eqs. (6)–(14), (26), and (27):

$$H_f^Q = \frac{e^2 B^2}{8m_e c^2} q^2 \tfrac{2}{3} \sqrt{4\pi} \left[Y_{00} - \frac{1}{\sqrt{5}} Y_{20} \right] , \tag{57}$$

where Y_{00} and Y_{20} are spherical harmonics. The quadratic interaction for positronium is $H_f^Q/2$.

Here we use $h^{(1)} + H_f^L + H_f^Q$ in degenerate perturbation theory to remove the degeneracy among the eigenstates of $h^{(0)}$. The evaluation of the matrix elements of $h^{(1)} + H_f^L + H_f^Q$ is straightforward and the Hamiltonian matrix is diagonalized with the method of Jacobi rotations [37].

Figure 1 displays the Zeeman splittings for the $N=2$, $J=\frac{1}{2}$ levels of hydrogen. The energy eigenvalues for the $m_F=0$, $F=0,1$, $2\,^2S_{1/2}$ and $2\,^2P_{1/2}$ states of hydrogen are listed for incremental values of the magnetic field in Table V. The results that are presented here to eight significant digits are extremely accurate. The $n=2$ Lamb shift calculated here is 1057.845(11) MHz, in excellent agreement with the measured value of 1057.845(9) MHz of Lundeen and Pipkin [38]. Likewise the fine structure $(2P_{3/2}-2P_{1/2}=10\,968.679$ MHz) and the $1S$ hyperfine structure given by 1420.474 MHz are accurate to order $\alpha(Z\alpha)^4$. Similar tables listing all of the states of hydrogen up to $n=3$ have been deposited with the Physics Auxiliary Publication Service (PAPS) [39].

Figure 2 displays the Zeeman structure of the $n=2$ lev-

TABLE III. The $\alpha(Z\alpha)^4$ corrections to the Fermi-Breit interaction with anomalous magnetic moments.

Hydrogen		Positronium	
State	ΔE (MHz)	State	ΔE (MHz)
$1S_{1/2}$ $F=0$	8117.4516	$1S_0$	2840.3741
$1S_{1/2}$ $F=1$	8117.4371	$1S_1$	1563.5894
$2S_{1/2}$ $F=0$	1037.9762	$2S_0$	370.0832
$2S_{1/2}$ $F=1$	1037.9744	$2S_1$	210.4851
$2P$	4.0519	$2P$	-2.9075
$3S_{1/2}$ $F=0$	309.3229	$3S_0$	110.7449
$3S_{1/2}$ $F=1$	309.3223	$3S_1$	63.4566
$3P$	1.2005	$3P$	-0.8615
$3D$	1.2057	$3D$	0.3108

TABLE IV. Lamb-shift corrections for hydrogen not included in Table III and the Fermi-Breit interaction with anomalous magnetic moments.

State	ΔE (MHz)
$1S_{1/2}$	712.474 981
$2S_{1/2}$	89.084 398
$2P_{1/2}$	44.110 156
$2P_{3/2}$	14.470 424
$3S_{1/2}$	26.385 697
$3P_{1/2}$	13.071 087
$3P_{3/2}$	4.288 216
$3D_{3/2}$	6.606 627
$3D_{5/2}$	0.472 626

el positronium. The Zeeman shifts for the $2\,{}^1P_1$ and $2\,{}^3P_0$ states of positronium are presented in Table VI for comparison with the works of Grotch and Kashuba [9] and of Lewis and Hughes [12]. When comparing the results presented in Table VI with the work of Grotch and Kashuba [9] it is important to remember that the latter authors determined the zero-field splittings only to order α^4 while Lewis and Hughes [12] determined the zero-field splittings to order α^5, as was done here. The results presented here are in exact agreement with the results of Lewis and Hughes [12], but are presented to three more significant digits. We note that the eigenvalue tables of Lewis and Hughes [12] are not precise enough to display the relativistic corrections to the Zeeman effect. Tables similar to Table VI for all of the $n=1$, 2, and 3 states of positronium can also be found in the PAPS deposit [39].

VI. SUMMARY

The linear Zeeman Hamiltonian for hydrogenlike atoms derived here and presented in Eqs. (28)–(34) are correct to order $\alpha(Z\alpha)^2$ and correct to all orders in m_e/m_N. This Hamiltonian includes previously neglected radiative corrections of order $\alpha(Z\alpha)^2(m_e/m_N)^q$ $(q=0,1,\ldots,\infty)$ and recoil corrections of order $\alpha(Z\alpha)^2(m_e/m_N)^q$ $(q=1,\ldots,\infty)$. These additional contributions are seen to be important only for hydrogenlike atoms, most notably for the $2P$ states in which they are of the order of 10^{-7} MHz/G. Neglecting these new contributions we find that our Hamiltonian for neutral atoms in the presence of a uniform magnetic field (B) is unitarily equivalent to the Hamiltonian of Grotch and Hegstrom [10] to first order in B. In addition, there are contribu-

TABLE V. Zeeman levels for the $m_F=0$, $F=0.1$; $2\,{}^2S_{1/2}$ and $2\,{}^2P_{1/2}$ states of hydrogen. Energy listed in 10^9 Hz.

| B (G)	${}^2S_{1/2}$ F = 1	${}^2S_{1/2}$ F = 0	${}^2P_{1/2}$ F = 1	${}^2P_{1/2}$
0	−12.635 948	−12.458 389	−13.693 792	−13.634 629
200	−12.841 548	−12.252 788	−13.763 851	−13.567 766
400	−13.115 493	−11.978 842	−13.859 954	−13.481 248
600	−13.393 856	−11.700 477	−13.960 884	−13.396 284
800	−13.673 366	−11.420 965	−14.065 624	−13.313 877
1 000	−13.953 339	−11.140 989	−14.174 014	−13.234 167
1 200	−14.233 545	−10.860 780	−14.286 039	−13.157 142
1 400	−14.513 883	−10.580 437	−14.401 726	−13.082 747
1 600	−14.794 304	−10.300 011	−14.521 107	−13.010 908
1 800	−15.074 780	−10.019 529	−14.644 218	−12.941 547
2 000	−15.355 295	−9.739 008	−14.771 090	−12.874 583
2 200	−15.635 838	−9.458 458	−14.901 749	−12.809 933
2 400	−15.916 402	−9.177 886	−15.036 213	−12.747 514
2 600	−16.196 982	−8.897 298	−15.174 494	−12.687 246
2 800	−16.477 574	−8.616 697	−15.316 595	−12.629 049
3 000	−16.758 176	−8.336 085	−15.462 511	−12.572 844
3 200	−17.038 787	−8.055 463	−15.612 229	−12.518 557
3 400	−17.319 404	−7.774 836	−15.765 728	−12.466 112
3 600	−17.600 026	−7.494 202	−15.922 979	−12.415 439
3 800	−17.880 653	−7.213 563	−16.083 944	−12.366 468
4 000	−18.161 283	−6.932 920	−16.248 581	−12.319 131
4 200	−18.441 917	−6.652 272	−16.416 837	−12.273 364
4 400	−18.722 553	−6.371 622	−16.588 655	−12.229 105
4 600	−19.003 192	−6.090 968	−16.763 974	−12.186 294
4 800	−19.283 833	−5.810 312	−16.942 723	−12.144 872
5 000	−19.564 475	−5.529 653	−17.124 830	−12.104 784
5 500	−20.266 087	−4.827 997	−17.594 275	−12.010 056
6 000	−20.967 706	−4.126 331	−18.082 932	−11.922 565
6 500	−21.669 329	−3.424 656	−18.589 438	−11.841 613
7 000	−22.370 955	−2.722 973	−19.112 407	−11.766 577
7 500	−23.072 583	−2.021 285	−19.650 466	−11.696 897
8 000	−23.774 212	−1.319 591	−20.202 289	−1.632 074
8 500	−24.475 842	−0.617 892	−20.766 621	−11.571 662
9 000	−25.177 472	0.083 811	−21.342 290	−11.515 261
9 500	−25.879 102	0.785 518	−21.928 213	−11.462 514
10 000	−26.580 731	1.487 229	−22.523 402	−11.413 101
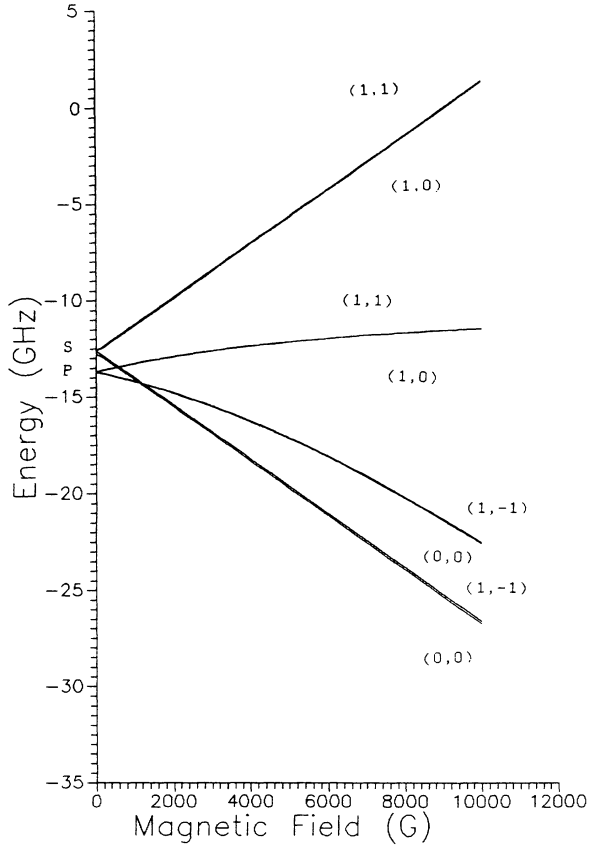
FIG. 1. Zeeman structure of the $n=2$, $J = \frac{1}{2}$ states of hydrogen. The numbers in parentheses are the quantum numbers (F, m_F). Nondegenerate traces which appear as one are labeled with the higher-energy state above the lower energy state.

FIG. 2. Zeeman structure of the $n=2$ states of positronium. The m_F quantum numbers are indicated.

tions for hydrogenlike ions $(Z \neq 1)$ of order $\alpha^2 m_e / m_N$ and $\alpha^3 m_e / m_N$ which are not included in the previous work [10]. However, when we take the matrix elements of these terms using the reduced mass, these contributions are seen to result in negligible corrections to the results of previous work which are smaller than $\alpha^3 m_e / m_N$.

Setting $m_e = m_N$ and $a_e = a_N$ the linear Zeeman interaction for positronium is obtained and is seen to be unitarily equivalent to the positronium Zeeman Hamiltonian obtained by Grotch and Kashuba [9] and by Lewis and Hughes [12].

The g factors presented in Sec. III are correct for all states of a two-body system of spin-$\frac{1}{2}$ particles with arbitrary atomic number Z. Excluding the effect of g_J, the g factors presented here agree with the g factors of Grotch and Kashuba [9] to one part in 10^{11}–10^{12}. The electronic-nuclear g-factor ratio for the ground state of hydrogen and the hydrogen-deuterium electronic g-factor ratio are consistently found to be $\simeq (1+2.8) \times 10^{-8}$ and $\simeq (1+7.2) \times 10^{-9}$, respectively, in any theoretical work on the Zeeman effect.

The tabulated results of the Zeeman shifts presented in Sec. V are extremely precise and are correct to order $\alpha(Z\alpha)^2$ and to all orders in m_e / m_N. It is the first time that such results have been computed for the $n=3$ states
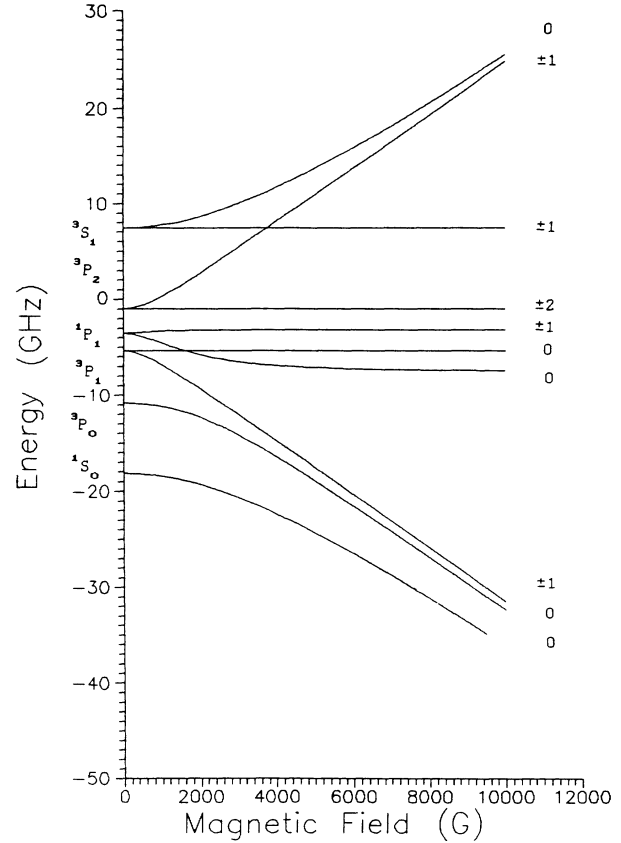
of hydrogen and positronium as far as we know. These results reflect the current knowledge of the zero-field structure of both hydrogen and positronium which is correct to order $\alpha(Z\alpha)^4$ and further utilizes the current theoretical knowledge of the Lamb shift in the case of hydrogen.

APPENDIX

In this appendix we show how we obtained the recoil correction in Eq. (20) and outline the evaluation of $\chi_z B$ from the sum of $H_{I3} + H_{I4}$. The reader is referred to Ref. [25] to see that we only need to consider the exchange of a single transverse photon between the electron and the nucleus in the presence of a constant external magnetic field to obtain the recoil correction for single-photon exchange. Introducing the magnetic field in the analysis of Ref. [25] is simply achieved by making the following substitution in Eq. (45) of Ref. [25]:

$$\frac{\mathbf{p}_i}{m_e} \rightarrow \frac{1}{m_e} \left[\mathbf{p}_e + \frac{e}{2} \mathbf{B} \times \mathbf{r}_e \right]_1 ,$$

$$-\frac{\mathbf{p}_i}{m_N} \rightarrow \frac{1}{m_N} \left[\mathbf{p}_N - \frac{e}{2} \mathbf{B} \times \mathbf{r}_N \right]_i . \tag{A1}$$

After retaining terms linear in the magnetic field, using the relations

$$\langle n|\mathbf{B}\times\mathbf{r}_e|n'\rangle = \frac{i}{m_e \Delta E_{n'n}}\langle n|\mathbf{B}\times\mathbf{p}_e|n'\rangle \ ,$$

$$\langle n'|\mathbf{B}\times\mathbf{r}_N|n\rangle = \frac{-i}{m_N \Delta E_{n'n}}\langle n'|\mathbf{B}\times\mathbf{p}_N|n\rangle \ ,$$ (A2)

summing over the polarization index (i), and integrating over the photon wave-vector direction we obtain Eq. (20).

To evaluate the radiative and recoil corrections of Eq. (34) we first make use of the commutation relations between r_e and $h^{(0)}$ and r_N and $h^{(0)}$ implicit in the derivation of Eq. (A2). We then get

$$\sum_{n'}\left[\frac{\langle n|\pi_x|n'\rangle\langle n'|\pi_y|n\rangle}{k+\Delta E_{n'n}}-\text{c.c.}\right]$$

$$=\sum_{n'}\left[\frac{\mu^2\Delta E_{n'n}^2\langle n|q_x|n'\rangle\langle n'q_y|n\rangle}{k\Delta E_{n'n}}-\text{c.c.}\right] \ .$$ (A3)

Expressing q_x and q_y in terms of the spherical components of q and using the Wigner-Eckart theorem the right-hand side of Eq. (A3) becomes

$$\sum_{n'}\sum_{L'}\sum_{m_1'}\frac{-i\mu^2\Delta E_{n'n}}{k+\Delta E_{n'n}}\left\{\frac{|\langle nLm_1=0|q_z|n'L'm_{1'}=0\rangle|^2}{\langle L'0;10L0\rangle\langle L0;10L'0\rangle}(\langle Lm_1;11L'm_1'\rangle-\langle Lm_1;1-1L'm_1'\rangle)\right.$$

$$\left.\times(\langle L'm_1';11Lm_1\rangle+\langle L'm_1';1-1Lm_1\rangle)\right\} \ .$$ (A4)

TABLE VI. Zeeman levels for the $2\,^1P_1$ and $2\,^3P_0$ states of positronium. Energy listed in 10^9 Hz.

B (G)	$^1P_1\ M_F=-1$	$^1P_1\ M_F=0$	$^1P_1\ M_F=+1$	$^3P_0\ M_F=0$
0	−3.538 612	−3.538 612	−3.538 612	−10.850 855
200	−3.515 649	−3.603 977	−3.515 649	−10.865 188
400	−3.461 755	−3.778 712	−3.461 755	−10.908 346
600	−3.402 207	−4.020 549	−3.402 207	−10.908 775
800	−3.351 026	−4.294 163	−3.351 026	−11.083 133
1 000	−3.311 343	−4.576 953	−3.311 343	−11.216 160
1 200	3.281 706	−4.855 340	−3.281 706	−11.380 520
1 400	−3.259 720	−5.121 143	−3.259 720	−11.576 624
1 600	−3.243 286	−5.369 471	−3.243 286	−11.804 464
1 800	−3.230 837	−5.597 618	−3.230 837	−12.063 505
2 000	−3.221 258	−5.804 436	−3.221 258	−12.352 644
2 200	−3.213 770	−5.989 927	−3.213 770	−12.670 256
2 400	−3.207 829	−6.154 914	−3.207 829	−13.014 304
2 600	−3.203 048	−6.300 769	−3.203 048	−12.382 485
2 800	−3.199 151	−6.429 177	−3.199 151	−13.772 380
3 000	3.195 935	−6.541 951	−3.195 935	−14.181 592
3 200	−3.193 254	−6.640 898	−3.193 254	−14.607 833
3 400	−3.190 995	−6.727 728	−3.190 995	−15.048 998
3 600	−3.189 075	−6.804 011	−3.189 075	−15.503 189
3 800	−3.187 429	−6.871 148	−3.187 429	−15.968 724
4 000	−3.186 006	−6.930 371	−3.186 006	−16.444 135
4 200	−3.184 769	−6.982 751	−3.184 769	−16.928 147
4 400	−3.183 684	−7.029 211	−3.183 684	−17.419 661
4 600	−3.182 728	−7.070 544	−3.182 728	−17.917 733
4 800	−3.181 880	−7.107 427	−3.181 880	−18.421 551
5 000	−3.181 124	−7.140 439	−3.181 124	−18.930 418
5 500	−3.179 552	−7.209 110	−3.179 552	−20.220 953
6 000	−3.178 320	−7.262 480	−3.178 320	−21.532 218
6 500	−3.177 328	−7.304 648	−3.177 328	−22.859 114
7 000	−3.176 508	−7.338 466	−3.176 508	−24.198 019
7 500	−3.175 816	−7.365 951	−3.175 816	−25.546 315
8 000	−3.175 219	−7.388 555	−3.175 219	−26.902 073
8 500	−3.174 694	−7.407 341	−3.174 694	−28.263 845
9 000	−3.174 224	−7.423 101	−3.174 224	−29.630 527
9 500	−3.173 796	−7.436 433	−3.173 796	−31.001 267
10 000	−3.173 400	−7.447 793	−3.173 400	−32.475 394

Using $q_z = q(4\pi/3)^{1/2}Y_{1,0}$, splitting the sum over states into its discrete and continuous parts, using Eq. (5.1.7) of Ref. [40], using the hydrogen wave functions in the coordinate representation, and integrating over all space we obtain for the bound states

$$|\langle nLm_1 = 0|q_z|n'L'm_1' = 0\rangle|^2$$

$$= \langle L'0;10L0\rangle^2\langle L0;10L'0\rangle^2 \frac{(n'-L'-1)!(n-L-1)!}{(n'+L')!^3(n+L)!^3 4n'n}$$

$$\times \left\{ \sum_{o=0}^{n-L-1} \sum_{p=0}^{n'-L'-1} (-1)^{o+p} \frac{(n+L)!^2(n'+L)!^2(L+L'+o+p+3)!}{(n-L-1-o)!(n'-L'-1-p)!o!p!(2L'+1+p)!(2L+1+o)!} \right.$$

$$\times \left. \left[\frac{1}{2} + \frac{n}{2n'}\right]^{-(L+L'+4+o+p)} \left[\frac{n}{n'}\right]^{L'+p} \right\}^2 \frac{1}{4}\frac{n^5}{n'^3} .$$ (A5)

The most convenient form of the hydrogen wave functions for the unbound states is given in Ref. [41]:

$$\psi_{\varepsilon,L,m_1}(q,\theta,\phi) = Y_{Lm_1}(\theta,\phi)\left[\frac{e^{2\pi z/k}-1}{2\pi^2 Z\prod_{i=1}^{L}\left[1+\frac{Z^2}{i^2\varepsilon}\right]}\right]^{1/2} \frac{e^{\pi z/k}i}{(2k)^L\Gamma(L+1)}\frac{q^L}{2}\int_{-ik}^{+ik}e^{xq}(x+ik)^{L+iz/k}(x-ik)^{L-iz/k}dz ,$$ (A6)

where $k = \sqrt{\varepsilon}$ and the product is replaced by unity for $L=0$. These wave functions are normalized such that

$$\int_\infty d\tau\,\psi_{\varepsilon2}^*\psi_{\varepsilon1} = \delta(\varepsilon1-\varepsilon2) .$$ (A7)

The sum over n' is now replaced by an integral over the energy parameter $\varepsilon = k^2 = 2E$. Integration over the angular coordinates produces the factor $\langle L'0;10L0\rangle^2\langle L0;10L'0\rangle^2$ as in Eq. (A5). A typical radial integral is

$$\int_0^\infty \psi_{2p}\psi_{\varepsilon s}q^3 dq$$

$$= \left[\frac{e^{2\pi/k}-1}{48\pi^2}\right]^{1/2}\frac{ie^{\pi/k}}{2}$$

$$\times \int_0^\infty dq\int_{-ik}^{+ik}dx\,q^4 e^{-(0.5-x)q}(x+ik)^{i/k}$$

$$\times (x-ik)^{-i/k} .$$ (A8)

Modifying the contour to pass around the barrier line connecting the branch points $x = \pm ik$ in the positive sense we pick up a factor of $(1-e^{2\pi z/k})$ and can legitimately interchange the order of integration. Integrating over dq and enclosing the resulting poles in the negative sense we get

$$\int_0^\infty \psi_{2p}\psi_{\varepsilon s}q^3 dq = \frac{-4!}{[48(1-e^{-2\pi/k})]^{1/2}}$$

$$\times \text{Res}\left[\frac{(x+ik)^{i/k}(x-ik)^{-i/k}}{(0.5-x)^5}\right] .$$ (A9)

Evaluating the residue at $x=0.5$ and after a little algebra we finally obtain

$$\int_0^\infty \psi_{2p}\psi_{\varepsilon s}q^2 dq = \frac{-e^{-2\vartheta/\sqrt{\varepsilon}}}{[48(1-e^{-2\pi/k})]^{1/2}}\frac{1}{\varepsilon^2(0.25+\varepsilon)^2}\{(2-22\varepsilon)\cos(4\vartheta)+(16-8)\cos(2\vartheta)+6(1+\varepsilon)$$

$$+\sqrt{\varepsilon}[12(1-\varepsilon)\sin(4\vartheta)-24\sin(2\vartheta)]\} ,$$ (A10)

where $\vartheta = \tan^{-1}(2\sqrt{\varepsilon})$. After evaluating the necessary radial integrals it is then possible to evaluate Eq. (A4) for any state $|n\rangle$. It is easier to integrate over the photon energy k before summing over the intermediate states. The integrals can be found in tables of integrals and numerical integration is not necessary. A computer program was used to evaluate the contribution from the sum over the bound states. The factorials in Eq. (A5) led to an extremely slow convergence of the results and it also limited the number of intermediate states that could be included to $n' < 90$ before reaching an overflow condition. However, from the definition of oscillator strengths $[f(nl,n')]$

$$|\langle nl|\pi_x|n'\rangle|^2 = \tfrac{1}{2}m_e(E_{n'}-E_n)f(nl,n') ,$$ (A11)

the known asymptotic $1/(n')^3$ dependence of oscillator strengths, $\sum_{n'=3}^{90}[1/(n')^3] = 0.076\,996$ and $\sum_{n'=3}^{10^{307}}[1/(n')^3] = 0.077\,056$, we are confident that the coefficients $[a(n,L,m_L)]$ in Eq. (35) are correct to five significant digits.

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[39] See AIP document no. PAPS PLRAAN-49-192-28 for 28 pages of the 20 tables displaying the Zeeman shifts for all of the $n = 1$, 2, and 3 states of hydrogen and positronium. Order by PAPS number and the journal reference from American Institute of Physics, Physics Auxiliary Publication Service, 500 Sunnyside Boulevard, Woodbury, NY 11797-2999. The price is $1.50 for each microfiche (60 pages) or $5.00 for photocopies of up to 30 pages and $0.15 for each additional page over 30 pages. Airmail additional. Make checks payable to the American Institute of Physics.

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