# Magnetic Interactions of One-Electron Atoms and of Positronium

H. Grotch and R. Kashuba

Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802

(Received 28 August 1972)

This paper constitutes a continuation of previous work on magnetic interactions of oneelectron atoms. In earlier papers the magnetic moment of a hydrogenic atom in its ground state was calculated, including radiative and nuclear-mass corrections. In this work the  $g_J$  and  $g_I$  factors are calculated for arbitrary hydrogenic states, including radiative and nuclear-mass corrections. The magnetic moment of a hydrogenic atom is obtained for any state. An extensive analysis of the Zeeman levels of positronium is carried out for the n=1and n=2 states, including higher-order corrections. For the n=1 state, the results confirm the validity of the Breit-Rabi formula with g factors in agreement with those given in an earlier paper by Grotch and Hegstrom. The annihilation diagram is included in the analysis but does not lead to any additional correction terms (to the accuracy we are working with). The Zeeman corrections in the n=1 state are relevant to the precise experimental determination of the positronium hyperfine structure. The analysis of the n=2 state Zeeman structure of positronium is similar to that carried out by Brodsky and Parsons for the n=2 states of hydrogenic atoms. Although the results in the hydrogenic case were immediately applicable to Lamb-shift measurements, the present results are not yet applicable since at present there is no experimental data on the excited states of positronium.

#### I. INTRODUCTION

In the past few years experiments have been performed to a high degree of precision to determine energy levels of one-electron atoms. The interpretation of these experiments requires a precise understanding of the Zeeman levels of such atoms; therefore, considerable theoretical effort has been expended to provide that understanding.

The theory of Zeeman levels in the n = 2 state of hydrogenic atoms, as discussed by Brodsky and Parsons<sup>1</sup> and Brodsky and Primack, <sup>2</sup> provides the oretical results needed in the precise experimental determinations of the Lamb shift. The work of Grotch and Hegstrom, <sup>3</sup> Faustov, <sup>4</sup> and Close and Osborn<sup>5</sup> on the bound-state corrections to g values in the ground state of hydrogenic atoms has been confirmed by measurements of  $g_e(H)/g_e(D)$ , and has also provided theoretical results needed for the recent precise determination of  $\mu_e/\mu_p$ , the ratio of magnetic moments of a free electron and a free proton.<sup>6</sup> This ratio appears in the theory of the hyperfine structure of hydrogen. Thus, a detailed understanding of Zeeman levels is a necessary ingredient in the continuing research on precision spectroscopy of one-electron atoms.

In this paper we extend previous work on Zeeman levels in several directions. The work of Grotch and Hegstrom is extended in Sec. II by evaluating explicitly the  $g_J$  and  $g_I$  factors for all states of hy-drogenic atoms with nuclear spin  $\frac{1}{2}$ . The corrections given include anomalous moment terms, binding corrections, and nuclear mass corrections linear in m/M. A simple formula is obtained explicitly for any state.

In Sec. III the Zeeman levels of the ground state of positronium are discussed. The annihilation diagram is incorporated in the zero-field Hamiltonian and is shown to produce a negligible effect on the magnetic field shifts. For the ground state, terms are calculated which are essential in the experimental measurement of the positronium hyperfine interval.

Section IV is an extension of the work of Brodsky and Parsons (n = 2 state of hydrogenic atoms) to the n = 2 states of positronium. In the case of hydrogen, correction terms of relative order  $(Z\alpha)^2m/M$  give very small contributions which were neglected in Ref. 1. In positronium, corresponding terms are of order  $\alpha^2$  since the mass ratio is unity. These additional terms are therefore needed in the analysis of Zeeman levels. At the present time, however, there are no experimental measurements in the n=2 state of positronium, although experimental groups are working on the problem. In Sec. V some conclusions are made concerning the relevance of these calculations to experiments.

## II. $g_J$ AND $g_I$ FACTORS FOR ALL STATES OF HYDROGENIC ATOMS

Grotch and Hegstrom<sup>3</sup> and others have calculated the magnetic moment of hydrogenic atoms in the ground state to very high accuracy. We have found, in this paper, that these results can be extended to any state of a hydrogenic atom. While our value for  $g_J$  will be completely general, independent of the value of the nuclear spin, the only restriction on the results concerns the higher-order corrections to  $g_I$ , which have only been calculated for a spin- $\frac{1}{2}$  nucleus.

7

7

The calculation of the g factors is accomplished by using Eq. (40) of Ref. 3. This equation was obtained by making a unitary transformation of the two-body Breit Hamiltonian (with anomalous moment interaction) in the presence of an external magnetic field. This unitary transformation was then followed by a Barker-Glover reduction as discussed fully in Ref. 3.

The corrections to g factors given here will contain only one power of m/M. Accordingly, the interaction Hamiltonian used will be H', where<sup>7</sup>

$$\begin{aligned} H' &= H'_{J} + H'_{I} = -\frac{e}{2m} \left( 1 - \frac{m}{M} - \frac{p^{2}}{2m^{2}} \right) \vec{L} \cdot \vec{H} \\ &- 2 \frac{e}{2m} \left\{ \vec{S} \cdot \vec{H} \left( 1 - \frac{\vec{p}^{2}}{2m^{2}} \right) + a_{e} \left( \vec{S} \cdot \vec{H} - \frac{\vec{S} \cdot \vec{p} \vec{p} \cdot \vec{H}}{2m^{2}} \right) \right. \\ &- V \left[ \frac{1}{4m} \left( 1 - \frac{2m}{M} \right) + \frac{a_{e}}{2m} \left( 1 - \frac{m}{M} \right) \right] \\ &\times (\vec{S} \cdot \vec{H} - \vec{S} \cdot \vec{r} \cdot \vec{r} \cdot \vec{H}) \right\} \\ &+ \frac{Ze}{2M} \left. 2 \left\{ (1 + a_{p}) \vec{I} \cdot \vec{H} + \frac{V}{Z} \left[ \frac{1}{2m} \left( 1 - \frac{m}{M} \right) \right. \\ &+ \frac{a_{p}}{2m} \left( 1 - \frac{m}{M} \right) \right] \left( \vec{I} \cdot \vec{H} - \vec{I} \cdot \vec{r} \cdot \vec{r} \cdot \vec{H} ) \right\} . \tag{1}$$

The terms involving  $\vec{L}$  and  $\vec{S}$  comprise  $H'_J$ , while those involving  $\vec{I}$  make up  $H'_I$ . The zero-field Hamiltonian includes a hyperfine interaction and therefore the unperturbed states are labeled by  $|nFm_FJL\rangle$ . Hereafter, it is understood that the nuclear spin is  $\frac{1}{2}$ , although this particular value has no effect on the  $g_J$  value. The  $g_J$  and  $g_I$  values may be defined by the relation

$$\langle nFm_{F}JL | H' | nFm_{F}JL \rangle$$

$$= \langle nFm_{F}JL | -\frac{e}{2m} g_{J} \vec{J} \cdot \vec{H}$$

$$+ \frac{Ze}{2M} g_{I} \vec{I} \cdot \vec{H} | nFm_{F}JL \rangle .$$
 (2)

The Wigner-Eckart theorem implies that  $g_{T}$  and  $g_I$  will be independent of  $m_F$ . Therefore, we may evaluate (2) by setting  $m_F = F$ . The terms in  $H'_J$ consist of operators which act only in a  $(J, m_J)$ representation. This implies that  $g_J$  may be evaluated in this representation. We readily find that

$$-(e/2m)g_J JH = \langle nJJLS | H'_J | nJJLS \rangle .$$
(3)

The value of spin S is always  $\frac{1}{2}$  since we are dealing with one-electron atoms. The matrix elements of the various vector operators appearing in (3) are easily evaluated. We find

$$\langle nJJLS | L_{z} | nJJLS \rangle = \frac{J(J+1) + L(L+1) - S(S+1)}{2(J+1)} ,$$
  
$$\langle nJJLS | S_{z} | nJJLS \rangle = \frac{J(J+1) - L(L+1) + S(S+1)}{2(J+1)} ,$$
  
$$\langle nJJLS | \vec{S} \cdot \hat{r} \hat{r}_{z} | nJJLS \rangle = \frac{\langle nJJLS | \vec{S} \cdot \hat{r} \hat{r} \cdot \vec{J} | nJJLS \rangle}{J+1} = \frac{1}{4(J+1)} ,$$
  
(4)

$$\langle nJJLS | \vec{S} \cdot \vec{p} \vec{p}_z | nJJLS \rangle = \frac{\langle nJJLS | \vec{S} \cdot \vec{p} \vec{p} \cdot \vec{J} | nJJLS \rangle}{J+1}$$
$$= \frac{1}{4(J+1)} \langle nJJLS | \vec{p}^2 | nJJLS \rangle.$$

From Eqs. (3) and (4) we readily obtain the value for  $g_J$ . The result, expressed in terms of the small quantities  $a_e$ ,  $\epsilon/m$ , and m/M is

$$g_{J} = \frac{3J(J+1) - L(L+1) + \frac{3}{4}}{2J(J+1)} - \frac{m}{M} \left( \frac{J(J+1) + L(L+1) - \frac{3}{4}}{2J(J+1)} \right) + \frac{\epsilon}{m} \left( \frac{4J(J+1) + 1}{4J(J+1)} \right) + \frac{\epsilon}{m} \frac{m}{M} \left( \frac{-3J(J+1) - L(L+1) - \frac{3}{4}}{2J(J+1)} \right) + a_{e} \left( \frac{J(J+1) - L(L+1) + \frac{3}{4}}{J(J+1)} \right) + a_{e} \frac{\epsilon}{m} \left( \frac{-2J(J+1) + 2L(L+1) + \frac{1}{2}}{2J(J+1)} \right) + a_{e} \frac{\epsilon}{m} \frac{m}{M} \left( \frac{4J(J+1) - 4L(L+1) - 1}{2J(J+1)} \right)$$
(5)

Here  $\epsilon$  is the nonrelativistic infinite-nuclear-mass binding energy  $-(m/2)(Z\alpha/n)^2$  and  $a_e = \frac{1}{2}(g_e - 2)$ , where  $g_e$  is the free-electron g factor. In (5) correction terms involving  $a_e(\epsilon/m)$  should contain only  $1 + (\alpha/2\pi)$  for the value of  $a_e$ , since we have not calculated binding corrections to higher-order terms in the anomalous moment of the electron.

The evaluation of  $g_I$  cannot be done in any subspace of the  $(F, m_F)$  space due to the presence in  $H'_I$  of the operator  $I \cdot \hat{r} \hat{r} \cdot \overline{H}$ . Therefore, we evaluate  $g_I$  directly. Using the Wigner-Eckart theorem we may extract from Eq. (2) the result

$$\frac{F(F+1)+I(I+1)-J(J+1)}{2(F+1)} g_I$$
$$= \langle nFFJL | C_1 I_s + C_2 \vec{1} \cdot \hat{\gamma} \hat{\gamma}_2 | nFFJL \rangle , \quad (6)$$

where

$$C_1 = 2(1+a_p) + \frac{2\epsilon}{mZ} \left[ \left( 1 - \frac{3m}{2M} \right) + \left( 1 - \frac{2m}{M} \right) a_p \right]$$

and

(9)

$$C_2 = -\frac{2\epsilon}{mZ} \left[ \left( 1 - \frac{3m}{2M} \right) + \left( 1 - \frac{2m}{M} \right) a_p \right] . \tag{7}$$

The matrix elements of  $I_a$  and of  $\mathbf{1} \cdot \hat{r} \hat{r}_a$  may be replaced by matrix elements of  $\mathbf{1} \cdot \mathbf{F}/(F+1)$  and  $\mathbf{1} \cdot \hat{r} \hat{r} \cdot \mathbf{F}/(F+1)$ , respectively. The matrix element of  $\mathbf{1} \cdot \mathbf{F}$  is trivial to evaluate. For nuclear spin  $\frac{1}{2}$  the operator  $\mathbf{1} \cdot \hat{r} \hat{r} \cdot \mathbf{F}$  is equal to  $\frac{1}{4} + \mathbf{1} \cdot \hat{r} \hat{r} \cdot \mathbf{S}$ . Therefore, the matrix elements of the scalar operator consisting of the scalar product of a vector operator in  $(I, m_I)$  space and a vector operator in  $(J, m_J)$  space are required. Using the 6j symbols this may be evaluated to obtain<sup>8</sup>

$$\langle nFFJL | \mathbf{\bar{I}} \cdot \hat{r} \, \mathbf{\bar{S}} \cdot \hat{r} | nFFJL \rangle$$

$$= (-1)^{J+I+F} \begin{cases} J & I & F \\ I & J & 1 \end{cases} \langle J || \mathbf{S}^{(1)} || J \rangle \langle I || I^{(1)} || I \rangle ,$$
(8)

where  $\langle J \| S^{(1)} \| J \rangle$  and  $\langle I \| I^{(1)} \| I \rangle$  are reduced matrix elements of the vector operators obtained from from  $\hat{r}(\mathbf{S} \cdot \hat{r})$  and  $\mathbf{I}$ , respectively. The reduced matrix elements are easily evaluated and are found to be

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

and

$$\langle J || s^{(1)} || J \rangle = \frac{1}{4} (2J+1)^{1/2} (J(J+1))^{-1/2}$$

We note that these reduced matrix elements turn out to be independent of L. This implies that the resulting  $g_I$  will be independent of orbital angular momentum and will therefore depend only on the atomic quantum numbers n and J; I is understood to be  $\frac{1}{2}$  throughout.

The 6*j* symbol given above is explicitly given in Edmonds.<sup>9</sup> Combining the various terms which contribute to  $g_I$  we obtained

$$g_{I} = C_{1} + \frac{C_{2}}{4J(J+1)} \left( \frac{J(J+1) - I(I+1) + F(F+1)}{F(F+1) - J(J+1) + I(I+1)} \right).$$
(10)

This expression is more conveniently written by factoring out  $2(1 + a_p)$ . We then obtained the final result;

$$g_{I} = 2(1+a_{p}) \left\{ 1 + \frac{\epsilon}{mZ} \left[ 1 - \frac{m}{2M} \left( \frac{3+4a_{p}}{1+a_{p}} \right) \right] \times \left[ 1 - \frac{1}{4J(J+1)} \left( \frac{J(J+1) - I(I+1) + F(F+1)}{F(F+1) - J(J+1) + I(I+1)} \right) \right] \right\}.$$
(11)

Equations (5) and (11) are in agreement with the ground-state results given in Ref. 3 and also are compatible with the  $g_J$  results given by Lamb<sup>10</sup> for the n = 2 states. The present results, however, contain additional terms beyond those already given by Lamb.

Finally, by combining the  $g_J$  and  $g_I$  results we may obtain a complete expression for the magnetic

moment of the hydrogen atom in any state. Using Eq. (2), the magnetic interaction may be replaced by

$$\left[ -\frac{e}{2m} g_{J} \left( \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)} \right) + \frac{Ze}{2M} g_{I} \left( \frac{F(F+1) - J(J+1) + I(I+1)}{2F(F+1)} \right) \right] \vec{F} \cdot \vec{H} \quad . \quad (12)$$

This result, which is quite fundamental, may be quite useful to experimentalists in the field of high-precision spectroscopy of one-electron atoms of nuclear spin  $\frac{1}{2}$ .

#### **III. POSITRONIUM**

The Zeeman structure of positronium will be examined by using the same formalism used to calculate the g factors. The two-component formalism based on the Breit Hamiltonian is correct except for terms of the order  $\vec{A}(\text{binding})^2/m^2$ . We have checked this conclusion, first arrived at by Brodsky and Primack from the Bethe-Salpeter equation.<sup>2</sup> In addition to those terms given in Eq. (40) of Ref. 3, we must include in the Hamiltonian the exchange interaction arising from the possibility of virtual-pair annihilation. The exchangeterm contribution is given by

$$H_{\rm ex} = \pi \, \frac{\alpha}{m^2} \, \bar{\mathbf{S}}^2 \, \delta(\mathbf{\hat{r}}) \,, \tag{13}$$

where  $\bar{S}$  is the total spin for positronium. We have examined the possibility of additional magneticfield corrections arising from  $H_{ex}$  in first-order perturbation theory by retaining magnetic-field corrections to the wave functions. These corrections turn out to be of order  $-(e/2m)H\alpha^4$  and are too small to be retained here.

If we retain only terms to first order in the external magnetic-field Hamiltonian we have for the field-dependent terms<sup>11</sup>

$$\begin{aligned} \mathcal{K} &= -\frac{e}{2m} \left[ \left( \vec{\sigma}_{e} - \vec{\sigma}_{p} \right) \cdot \vec{\mathrm{H}} \left( 1 - \frac{\mathbf{p}^{2}}{2m^{2}} \right) \right. \\ &+ a_{e} \left( \left( \vec{\sigma}_{e} - \vec{\sigma}_{p} \right) \cdot \vec{\mathrm{H}} - \frac{\left( \vec{\sigma}_{e} - \vec{\sigma}_{p} \right) \cdot \vec{\mathrm{p}} \cdot \vec{\mathrm{p}} \cdot \vec{\mathrm{H}}}{2m^{2}} \right) \right] \\ &+ \frac{e \, \alpha}{8m^{2}} \left( \frac{\left( \vec{\sigma}_{e} - \vec{\sigma}_{p} \right) \cdot \vec{\mathrm{H}} \, r^{2} - \left( \vec{\sigma}_{e} - \vec{\sigma}_{p} \right) \cdot \vec{\mathrm{r}} \, \vec{\mathrm{r}} \cdot \vec{\mathrm{H}}}{r^{3}} \right) . \end{aligned}$$
(14)

The calculation of the Zeeman levels is done using first-order perturbation theory. The basic unperturbed Hamiltonian  $H_0$  for positronium is the same as for the nonrelativistic Coulomb problem except with a reduced mass  $\frac{1}{2}m$ . We may evaluate the fine-structure corrections, based on Eq. (40) of Ref. 3 plus the annihilation term of Eq. (13), by means of first-order perturbation theory, since these terms are smaller by two powers of  $\alpha$ . Next, consider the terms proportional to the magnetic field, given by Eq. (14). Since the orbital magnetic moment of positronium is equal to zero, and the spin-magnetic-moment operator is proportional to the difference of the spins, all matrix elements  $\langle S, M_S | \mathcal{K} | S', M'_S \rangle$  vanish with the exception of  $\langle 0, 0 | (\sigma_e - \sigma_p)_z | 1, 0 \rangle$  and  $\langle 1, 0 | (\sigma_e - \sigma_p)_z | 0, 0 \rangle$ . Since  $L^2$  and  $M_F$  remain good quantum numbers, we will examine  $\mathcal{K}$  between states  $|LSFM_F\rangle$  diagonal in L and  $M_J$ .

### Zeeman Structure of the Ground State

In the ground state the magnetic-field Hamiltonian connects the  $M_J = 0$  components of the singlet and triplet states. The triplet states with  $M_F = \pm 1$ are unaffected by the presence of the field. The characteristic values are given by

$${}^{3,1}E = \frac{1}{2} ({}^{3}W + {}^{1}W) \pm \left[\frac{1}{4} ({}^{3}W - {}^{1}W)^{2} + \langle \mathcal{K} \rangle^{2}\right]^{1/2} .$$
(15)

Here  ${}^{3,1}E$  denotes the M=0 energies of ortho- and parapositronium, respectively. The energies  ${}^{1}W$ ,  ${}^{3}W$  are the fine-structure corrections to the Schrödinger energy level. Our calculated values for these quantities are given by

$$^{1}W = -\frac{21}{64} m \alpha^{4}$$
, (16a)

$$^{3}W = {}^{1}W + \frac{7}{12} m \alpha^{4}$$
 (16b)

As stated above the only nonvanishing matrix element of  $\mathcal{K}$  is between the state  $|LSFM_F\rangle = |0110\rangle$ and  $|0000\rangle$ . If we denote the expectation value of the magnetic-field-dependent terms by  $\langle \mathcal{K} \rangle$  we have

$$\langle \mathfrak{K} \rangle = -(e/m) H (1 + a_e - \frac{5}{24} \alpha^2 - \frac{1}{24} a_e \alpha^2) .$$
 (17)

Note that for the ground state this matrix element may be obtained from the g-factor calculation given by Grotch and Hegstrom.<sup>3</sup>

As reported by Carlson, Hughes, and Theriot, <sup>12</sup> experiments are in progress to determine the finestructure separation of the ground state of positronium to about 10 ppm. We shall show that this more accurate determination of g is important for measurements of this precision. As reported by the aforementioned authors, the measurement of the fine structure by inducing a direct transition between the  ${}^{3}S_{1}$  and  ${}^{3}S_{0}$  states is difficult. However, the separation  $\nu = {}^{3}S_{1} - {}^{1}S_{0}$  can be measured by inducing a transition between the  $M_{F} = 0$  and  $M_{F}$  $= \pm 1$  levels of orthopositronium. From the Breit-Rabi formula Eq. (15), but with measured values for the W's, we obtain for the frequency of this transition

$$f = {}^{3}E - {}^{3}W = \frac{1}{2}\nu\left\{ \left[ 1 + \left( bg^{2}/\nu^{2} \right) \right]^{1/2} - 1 \right\},$$
(18)

where  $b \equiv 4 \mu_B^2 H^2$ , g is the electron g factor, and  $\mu_B$  is the Bohr magneton.

We want to examine how sensitive the measured

value of  $\nu$  is to the determination of g. If we solve Eq. (18) for  $\nu$  we obtain

$$\nu = (bg^2 - 4f^2)/4f . \tag{19}$$

Thus the precision of  $\nu$  depends on the experimental determination of b and f, and the theoretical value of g. As a function only of the theoretical g [Eq. (19)] gives

$$\frac{\Delta\nu}{\nu} = \left(\frac{2bg^2}{bg^2 - 4f^2}\right) \frac{\Delta g}{g} \quad . \tag{20}$$

The measurement of Carlson, Hughes, and Theriot was done at 7900 G and the Zeeman frequency is about 2.4 GHz. If  $\Delta g = 2 \times \frac{5}{24} \alpha^2$  we find that  $\Delta \nu / \nu \simeq 11 \times 10^{-6}$  or 11 ppm. Now if we had used the old value of  $\frac{1}{3}$  instead of  $\frac{5}{24}$  the difference would have lead to a fractional error in  $\Delta \nu / \nu$  of about 7 ppm.

## IV. ZEEMAN STRUCTURE OF THE n = 2 STATE

For the n=2 state, but with zero orbital angular momentum, we have essentially the same situation as for the ground state. We only have splitting for the  $M_F = 0$  components of the singlet and triplet states. The characteristic values are again given by Eq. (15), but this time

$${}^{1}W = -\frac{53}{1024} m\alpha^4 , \qquad (21a)$$

$$W = {}^{1}W + \frac{7}{96} m \alpha^{4} , \qquad (21b)$$

and

3

$$\langle 3C \rangle = -(e/m) H(1 + a_e - \frac{5}{96} \alpha^2 - \frac{1}{96} a_e \alpha^2)$$
. (21c)

For the states n=2 and L=1, the states which are connected by the magnetic-field-dependent terms have the same value of  $M_F$  and have  $\Delta S = 1$ . Thus for the case where  $M_F = \pm 1$ , the states  $|112\pm1\rangle$  and  $|111\pm1\rangle$  connect with  $|101\pm1\rangle$ , and for  $M_F = 0$  we may have  $|1120\rangle$ ,  $|1110\rangle$ ,  $|1100\rangle$  connecting with  $|1110\rangle$ . However, the matrix element of  $\mathcal{K}$  between  $|1110\rangle$  and  $|1010\rangle$  has zero magnitude, so again we have two states coupled to a third by the magnetic-field-dependent term. All other P states are unaffected by the magnetic field. In each of the above cases we have a third-order characteristic equation to solve for the eigenvalues. If we label two of the above states by 2 and 1 and the third state by 0, then the characteristic equation can be written as the determinant

$$\begin{array}{c|c} (E^{i} - {}^{2}W) & 0 & -\langle 2 | \Im C | 0 \rangle \\ 0 & (E^{i} - {}^{1}W) & -\langle 1 | \Im C | 0 \rangle \\ -\langle 0 | \Im C | 2 \rangle & -\langle 0 | \Im C | 1 \rangle & (E^{i} - {}^{0}W) \end{array} = 0 .$$
 (22)

For  $M_F = \pm 1$  we have  ${}^2W = {}^3P_2$ ;  ${}^1W = {}^3P_1$ ;  ${}^0W = {}^1P_1$ and

$$\langle 2 | \mathcal{K} | 0 \rangle = \langle 112 \pm 1 | \mathcal{K} | 101 \pm 1 \rangle$$
  
=  $-(1/\sqrt{2})(e/m) H (1 + a_e - \frac{1}{20} \alpha^2 - \frac{1}{80} a_e \alpha^2) , \quad (23a)$ 

$$\langle 1 | \mathcal{K} | 0 \rangle = \langle 111 \pm 1 | \mathcal{K} | 101 \pm 1 \rangle$$
  
=  $-\pm (1/\sqrt{2}) (e/m) H (1 + a_e - \frac{1}{16} \alpha^2) .$  (23b)  
For  $M_F = 0$  we have  ${}^2W = {}^3P_2$ ,  ${}^1W = {}^3P_0$ ,  ${}^0W = {}^1P_1$  and  $\langle 2 | \mathcal{K} | 0 \rangle = \langle 1120 | \mathcal{K} | 1010 \rangle$ 

$$= -\frac{2}{3} (e/m) H (1 + a_e - \frac{9}{160} \alpha^2 + \frac{1}{160} \alpha^2 a_e) , \quad (24a)$$

 $\langle 1 | \mathcal{H} | 0 \rangle = \langle 1100 | \mathcal{H} | 1010 \rangle$ 

$$= -(1/\sqrt{3})(e/m)H\left[-1-a_e+\frac{1}{16}\alpha^2-\frac{1}{32}\alpha^2(1-a_e)\right].$$
(24b)

The calculated values of the fine structure are given by  $% \left( \frac{1}{2} \right) = 0$ 

$${}^{3}P_{2} = -\frac{31}{3072} m \alpha^{4} + \frac{7}{960} m \alpha^{4} , \qquad (25a)$$

$${}^{3}P_{1} = -\frac{31}{3072} m \alpha^{4} - \frac{1}{192} m \alpha^{4} , \qquad (25b)$$

$${}^{3}P_{0} = -\frac{31}{3072} m \alpha^{4} - \frac{1}{48} m \alpha^{4} , \qquad (25c)$$

$${}^{1}P_{1} = -\frac{31}{3072} \ m\alpha^{4} \ . \tag{25d}$$

The solutions of the two cubic equations which arise

from Eq. (22) have been obtained for values of H up to 1 T. These are listed in Table I and shown on Fig. 1. In the numerical calculations, we have used the values of the fundamental constants given by Taylor, Parker, and Langenberg.<sup>13</sup>

### V. CONCLUSIONS

The results obtained in Secs. I–IV should prove useful in the precision spectroscopy of one-electron atoms and also in other situations such as muonic atoms in which the electrons present constitute a small perturbation on the muonic levels.

The g factors in the 2S state of hydrogen could be useful in a determination of  $\mu_e/\mu_p$ , the ratio of electron-to-proton magnetic moments. In Ref. 6 this quantity was determined by simultaneous measurement of electronic and nuclear magnetic transition frequencies. As noted, the nuclear moment interacts much more strongly with the electron moment than with the external field. Due to this, to achieve a given over-all precision in the determination of  $\mu_e/\mu_p$ , the proton transition must be measured to a much higher precision than the electron transition. If the corresponding experiment

TABLE I. Solutions of the two cubic equations which arise from Eq. (22). Energy listed is in  $10^9$  Hz.

H (tesla)	$M_{F}^{=\pm 1}_{{}^{3}P_{2}}$	$M_F = \pm 1$ <sup>1</sup> P <sub>1</sub>	$M_F = \pm 1 \\ {}^{3}P_1$	$M_{F} = 0$ ${}^{3}P_{2}$	$M_{F} = 0$ ${}^{1}P_{1}$	$M_F = 0$ ${}^{3}P_0$
0.00	-0.9809	-3,5357	-5.3606	-0.9809	-3.5357	-10.8352
0.02	-0.9200	-3.5127	-5.4444	-0.9011	-3.6012	-10.8496
0.04	-0.7442	-3.4589	-5.6740	-0.6829	-3.7761	-10.8928
0.06	-0.4714	-3.3994	-6.0063	-0.3684	-4.0181	-10.9654
0.08	-0.1237	-3.3483	-6.4051	0.0079	-4.2918	-11.0679
0.10	0.2786	-3.3088	-6.8470	0.4239	-4.5745	-11.2012
0.12	0.7196	-3.2792	-7.3176	0.8669	-4.8528	-11.3659
0.14	1.1881	-3.2573	-7.8080	1.3290	-5.1184	-11.5623
0.16	1.6763	-3.2410	- 8.3125	1.8053	-5.3665	-11.7906
0.18	2.1787	-3.2286	-8.8273	2.2927	-5.5944	-12.0501
0.20	2.6918	-3.2190	-9.3500	2.7888	-5.8008	-12.3397
0.22	3.2130	-3.2116	-9.8786	3.2920	-5.9860	-12.6579
0.24	3.7405	-3.2057	-10.4119	3.8012	-6.1506	-13.0024
0.26	4.2728	-3.2010	-10.9490	4.3154	-6.2961	-13.3711
0.28	4.8090	-3.1971	-11.4890	4.8338	-6.4241	-13.7615
0.30	5.3484	-3.1939	-12.0317	5.3559	-6.5366	-14.1712
0.32	5.8904	-3.1913	-12.5763	5.8812	-6.6352	-14.5979
0.34	6.4346	-3.1890	-13.1227	6.4094	-6.7217	-15.0394
0.36	6,9806	-3.1872	-13.6706	6.9400	-6.7978	-15.4940
0.38	7.5280	-3.1855	-14.2197	7.4728	-6.8647	-15.9599
0.40	8,0768	-3.1842	-14.7698	8,0075	-6.9237	-16.4356
0.42	8.6267	-3.1830	-15.3209	8.5440	-6.9759	-16.9199
0.44	9.1776	-3.1819	-15.8729	9.0822	-7.0222	-17.4117
0.46	9.7293	-3.1810	-16.4255	9.6217	-7.0634	-17.9101
0.48	10.0282	-3.1802	-16.9789	10.1625	-7.1002	-18.4141
0.50	10.8348	-3.1794	-17.5325	10.7046	-7.1331	-18,9232
0.60	13.6077	-3.1768	-20.3080	13.4291	-7.2550	-21.5259
0.70	16.3890	-3.1752	-23.0910	16.1717	-7.3310	-24.1925
0.80	19.1757	-3.1742	-25.8787	18.9266	-7.3813	-26.8971
0.90	21.9660	-3.1735	-28,6696	21.6905	-7.4160	-29.6261
1.00	24.7586	-3.1730	-31.4628	24.4611	-7.4410	-32.3715



FIG. 1. Zeeman levels for n=2 states of positronium.

could be done in the n=2 state, the hyperfine interaction would be diminished by a factor of  $\frac{1}{8}$  while the proton coupling to the external field would be essentially unaffected. Thus, to achieve a given precision in  $\mu_e/\mu_p$  one could get away with a less accurate determination of the proton resonance frequency in the n=2 state. Alternatively, it might be possible to make a more precise determination of  $\mu_e/\mu_p$  in the n=2 state.

The determination of  $g_J$  and  $g_I$  values in Sec. II contains correction terms of order  $(Z\alpha)^2$ ,  $\alpha(Z\alpha)^2$ ,  $(Z\alpha)^2m/M$ , and  $\alpha(Z\alpha)^2m/M$  for all states of hydrogenic atoms. In these expressions the factor of  $\alpha$  arises from the anomalous magnetic moment of the electron (or muon for muonic atoms). However, if the atom is more exotic, such as an antiproton bound to a heavy nucleus, then the factor  $\alpha/2\pi$  may be replaced by the appropriate anomalous moment. In atoms of this type, with high Z, some of the correction terms to Zeeman shifts are as large as the basic Zeeman interaction itself. However, in these systems Zeeman shifts are extremely small when compared to the basic level spacing.

As previously discussed our ground-state results

for positronium are useful in the experimental determination of the hyperfine splitting of positronium. Terms neglected in our g-factor calculation should be of order  $\alpha^4$  and smaller, and therefore the g factor is known to very high accuracy.

The results for the excited states of positronium have been tabulated and also plotted. It is interesting to note that the  $M_F = \pm 1$  levels remain degenerate in all cases. The matrix elements of  $\mathcal{H}$  are diagonal with respect to the  $M_r$ , and those involving +1 are either equal to or the negative of those involving -1 [see Eqs. (23a) and (23b)]. Since the characteristic equation, Eq. (22), will only involve the squares of these matrix elements, the equations are identical for both  $M_F$  values. We note also that the  $M_F = 0$  level is quite close to the  $M_F$  $=\pm 1$  levels in the  ${}^{3}P_{2}$  state and that these levels cross at about 0.32 T. We have not found any simple explanation for the closeness of these levels but rather think it is accidental, being more a consequence of the specific spacing of the zero-field levels than of any symmetry.

At the present time there are no experiments which have been done in the n = 2 states of positronium. Since this system is so fundamental, it would be quite valuable to study these states both theoretically and experimentally. There are at present several experimental groups attempting to form and study these levels.

Note added in proof. In this paper we have not included the finite corrections of order  $\alpha(Z\alpha)^2$  and  $\alpha(Z\alpha)^2 m/M$  to  $g_I$  and  $g_J$  arising from terms discussed in Ref. 7. Such corrections appear to exist for  $l \neq 0$ . The calculation of these terms appears difficult due to the sum on states, and the results are unimportant at present. They may be computed numerically by using Coulomb Green's functions, but a different numerical calculation is required for each state. As a result, Eqs. (5), (11), and (12) do not contain all corrections of order  $\alpha(Z\alpha)^2$  and  $\alpha(Z\alpha)^2 m/M$  for states with nonzero angular momentum. When this work was completed we learned that similar results for Zeeman interactions of positronium were also obtained by Lewis and Hughes [see M. L. Lewis and V. W. Hughes, in Abstracts of the Third International Conference on Atomic Physics, Boulder, Colorado, August, 1972 (unpublished), p. 149].

### ACKNOWLEDGMENT

One of us (H.G.) would like to thank Professor Santiago R. Polo for valuable discussions.

- <sup>4</sup>R. Faustov, Phys. Letters <u>33B</u>, 422 (1970).
- <sup>5</sup>F. E. Close and H. Osborn, Phys. Letters 34B, 400

<sup>&</sup>lt;sup>1</sup>S. J. Brodsky and R. G. Parsons, Phys. Rev. <u>163</u>, 134 (1967).

<sup>&</sup>lt;sup>2</sup>S. J. Brodsky and J. R. Primack, Ann. Phys. (N. Y.) <u>52</u>, 315 (1969).

 $<sup>^{3}\</sup>mathrm{H.}$  Grotch and R. A. Hegstrom, Phys. Rev. A  $\underline{4},$  59 (1971).

(1971).

<sup>6</sup>P. F. Winkler, D. Kleppner, T. Myint, and F. G. Walther, Phys. Rev. A 5, 83 (1972).

<sup>7</sup>This Hamiltonian includes only the anomalous moment interaction based on  $\Delta E_n(M)$ , Eq. (3) of Ref. 1. However, Eq. (A4) of Ref. 1 (and references cited therein) suggest another level shift

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

where  $H - E_n = (1/2m)(m^2 - \pi^2)$ . This is also due to radiative corrections. The magnetic field dependence of this expression can come from field dependence of  $H - E_n$  or from the factors of  $\pi_{\mu}$ . The dependence of the first type is proportional to

$$\sum_{n'} \langle n | \vec{p} | n' \rangle \cdot \frac{\Delta E_{n'n}^{H}}{\Delta E_{n'n}} \langle n' | \frac{\vec{r}}{r^{3}} | n \rangle$$

to first order in the magnetic field, where  $\Delta E_n^{H}$  is the difference of magnetic shifts of states  $|n\rangle$  and  $|n'\rangle$  while  $\Delta E_{n,n}$  is the zero-field energy difference. At this stage of the calculation the states are taken to be eigenstates of  $H_{NR}$  and may also be taken as eigenstates of the magnetic part of  $H_{NR}$  as well as the zero-field part of  $H_{NR}$ . The above can then be written

$$\sum_{n'} im \langle n | \vec{\mathbf{r}} | n' \rangle \cdot \Delta E_{n'n}^{H} \langle n' | \frac{\vec{\mathbf{r}}}{r^{3}} | n \rangle = im \langle n | [\vec{\mathbf{r}}, H_{\text{mag}}] \cdot \frac{\vec{\mathbf{r}}}{r^{3}} | n \rangle.$$

This reduces to a matrix element of  $(\vec{r} \times \vec{H}) \cdot \vec{r}$  and therefore vanishes. The contribution to  $\Delta E_n(L)$  from terms of the second type may be shown to be

$$-\frac{\alpha ei}{3\pi m^3} \int_0^\infty \frac{dk}{1+2k/m} \ \vec{\mathrm{H}} \cdot \sum_{n'} \frac{\langle n | \vec{\mathfrak{p}} | n' \rangle \times \langle n' | \vec{\mathfrak{p}} | n \rangle}{k + \Delta E_{n'n}}$$

For S states the  $|n'\rangle$  sum will lead to a spin-independent result. Therefore, the result must vanish since it can only be proportional to  $l_z$  which is zero. For states with  $l \neq 0$  it appears that finite corrections of order  $\alpha (Z\alpha)^2$ and  $\alpha(Z\alpha)^2 m/M$  are possible. Subsequent equations, Eqs. (5), (11), and (12) do not, therefore, contain all corrections of order  $\alpha (Z\alpha)^2$  and  $\alpha (Z\alpha)^2 m/M$  for states with  $l \neq 0$ . See also the Note added in proof.

<sup>8</sup>K. Gottfried, Quantum Mechanics (Benjamin, New York, 1966), Vol. 1, p. 305.

<sup>9</sup>A. R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton U. P., Princeton, N. J., 1957), p. 130. <sup>10</sup> W. E. Lamb, Jr., Phys. Rev. <u>85</u>, 259 (1952).

<sup>11</sup>Even though the Zeeman levels depend on  $H^2$  the terms in the Hamiltonian which are quadratic in the magnetic field produce an energy shift of only about 10<sup>5</sup> Hz. This is of the same order as other terms not included here. This Hamiltonian again includes only the anomalous moment interactions. Other radiative corrections (see Ref. 7 above), negligible for the hydrogen atom, also appear to be too small in positronium.

<sup>12</sup>E. R. Carlson, V. W. Hughes, and E. D. Theriot, Jr., in Precision Measurements and Fundamental Constants, Natl. Bur. Std. (U.S.) Spec. Publ. No. 343 (U.S. GPO, Washington D. C., 1971).

<sup>13</sup>B. N. Taylor, W. H. Parker, and D. N. Langenberg, Rev. Mod. Phys. 41, 375 (1969).