## Higher-Order Relativistic Contributions to the Zeeman Effect in Helium\*

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A calculation of higher-order relativistic contributions to the Zeeman effect in the  $2^{3}P$ ,  $2^{3}S$ ,  $3^{3}P$ ,  $4^{3}P$ , and  $5^{3}P$  states of helium is given. The contributions to the g factors  $g'_{S}, g'_{L}$ , and  $g_{X}$ , have been calculated to order  $\alpha^{2}$  and m/M where m is the electron mass and M is the helium mass. Relativistic contributions are obtained from the matrix elements of a reduced Breit Hamiltonian with a series of numerical wave functions using a Hylleraas basis. The comparison of the theoretical values with the experimental determinations of the g factors is given for the  $2^{3}P$  and  $2^{3}S$  states. The value of  $g'_{S}$  calculated for  $2^{3}P$  helium is within two standard deviations of the experimental error of the measurement of Lewis *et al.* A recent precise measurement of the g factor in  $2^{3}S_{1}$  helium by Brossel *et al.* is three standard deviations of the experimental error from the value calculated here and from the result of Perl and Hughes. These higher-order contributions are necessary for the determination of the  $2^{3}P$  fine-structure intervals from the Zeeman effect, and hence to test the theory of fine structure for helium and to  $d_{1}$  and precisely the fine-structure constant  $\alpha$  from the helium fine structure. The relativistic contributions to  $g'_{S}$  have been calculated for the helium isoelectronic series from Li II through Ne IX for the  $2^{3}P_{1}$ ,  $3^{3}P_{1}$ ,  $4^{3}P_{1}$ , and  $5^{3}P_{1}$  states.

#### I. INTRODUCTION

Higher-order relativistic contributions to the theory of atomic magnetism for two-electron atoms are of intrinsic interest. Also, higherorder contributions to the Zeeman effect in helium are needed for the precise determination of the  $2^{3}P$  fine-structure intervals and for a determination of the fine-structure constant  $\alpha$  from the measurement of the energy levels of the  $2^{3}P$  state in a magnetic field.<sup>1,2</sup> In this paper the contributions to the Zeeman effect are calculated to order  $\alpha^2 \mu_B H$  and  $(m/M) \mu_B H$ , where m is the electron mass and M is the helium atom mass, for the  $2^{3}P$ ,  $2^{3}S$ ,  $3^{3}P$ ,  $4^{3}P$ , and  $5^{3}P$  states of  $^{4}\text{He}.^{3-5}$ The relativistic contributions to  $g_s$  for the  $2^{3}P_1$ ,  $3^{3}P_{1}$ ,  $4^{3}P_{1}$ , and  $5^{3}P_{1}$  states of the helium isoelectronic series from Li II through Ne IX are given.

The Hamiltonian for the Zeeman effect includes terms to order  $\alpha^2$  and m/M for helium and contains both relativistic and virtual radiative contributions to atomic magnetism.<sup>6-8</sup> The way anomalous moments and relativistic contributions to the g factors combine in a composite system<sup>9</sup> is of interest. Discrepancies are present between the theoretically and experimentally determined g factors for some many-electron atoms.<sup>10</sup>

The comparison of theoretical and experimental values<sup>1,2,11,12</sup> of the fine-structure intervals and the Zeeman effect in the  $2^{3P}$  state of helium is a significant test of the theory of two-electron atoms. It is of particular interest to test the two-body wave equation in states of nonzero orbital angular momentum since many terms in the Hamil-

tonian that vanish for S states are nonzero in P states.

The Zeeman Hamiltonian, accurate to order  $\alpha^2$ , was developed from a modified Breit equation<sup>13</sup> by Perl and Hughes,<sup>6</sup> Abragam and Van Vleck,<sup>14</sup> and Kambe and Van Vleck.<sup>15</sup> Many similar operators appear in the fine-structure Hamiltonian and hence the fine-structure interval may be calculated by methods used here.<sup>16</sup>

A precise evaluation of the matrix elements of the Zeeman Hamiltonian requires an adequate atomic wave function. A series of numerical wave functions in a Hylleraas basis is calculated.<sup>16</sup> The extrapolated value of the energy from the calculation of the wave function is accurate to better than one part in  $10^7$ . Ten wave functions for the  $2^{3}P$  state with 1, 2, 4, 10, 20, 35, 56, 84, 120, and 165 terms are each used to obtain matrix elements of the Zeeman Hamiltonian.

A discrepancy of three standard deviations of the experimental error exists between a new higher-precision experimental  $g_J$  value for  $2 \, {}^3S_1$ helium by Brossel *et al.*<sup>17</sup> and the previous calculation<sup>6</sup> and experiment.<sup>18</sup> In an attempt to verify and improve the calculation by Perl and Hughes<sup>6</sup> of the  $g_J$  factor in the  $2 \, {}^3S_1$  state of helium, we have recalculated the Zeeman effect in that state.

In Sec. II the Zeeman Hamiltonian  $\mathcal{K}_z$  and its reduction are presented. A discussion of numerical wave functions for  $2^{3}P$  and  $2^{3}S$  helium is given in Sec. III. In Sec. IV the results and discussion of the relativistic contributions to the Zeeman effect in triplet states in helium and heliumlike ions are presented. The Appendix gives an expansion of the interelectron distance in terms of

hypergeometric functions and Legendre polynomials. Brief reports of this research have been presented.<sup>3,5</sup>

#### **II. ZEEMAN HAMILTONIAN**

The Zeeman Hamiltonian for helium can be developed from the Breit equation.<sup>19</sup> The theoretical development of the reduced Hamiltonian was due to Perl and Hughes,<sup>6</sup> Abragam and Van Vleck,<sup>14</sup> and Kambe and Van Vleck.<sup>15</sup> Innes and Ufford<sup>20</sup> re-expressed the Zeeman Hamiltonian in spherical-tensor notation.<sup>21</sup> The use of spherical tensors greatly facilitates the calculation of the g factors.<sup>20</sup>

#### A. The Breit Equation

In order to apply the theory to more general cases than two-electron atoms, we write the Breit equation<sup>13</sup> as

$$\mathcal{K}_{B} = \sum_{i} \left( \vec{\alpha}_{i} \cdot \vec{p}_{i} + \beta_{i} m - Z e^{2} / r_{i} \right) + e^{2} \sum_{i < j} \left( \frac{1}{r_{ij}} - \frac{\vec{\alpha}_{i} \cdot \vec{\alpha}_{j}}{2r_{ij}} - \frac{\vec{\alpha}_{i} \cdot \vec{r}_{ij} \vec{\alpha}_{j} \cdot \vec{r}_{ij}}{2r_{ij}^{3}} \right),$$

$$(2.1)$$

where for helium the sum is over two electrons. In  $\mathcal{R}_{B}$ ,  $\mathbf{\bar{r}}_{i}$  is the position of the *i*th electron,  $\mathbf{\bar{p}}_{i}$  is the momentum,  $\mathbf{\bar{\alpha}}_{i}$  and  $\beta_{i}$  are the Dirac matrices, *m* is the electron mass, *e* is the electron charge, and  $\hbar = c = 1$ . In the presence of an external magnetic field,  $\mathbf{\bar{p}}_{i}$  is replaced by  $\mathbf{\bar{p}}_{i} + e \mathbf{\bar{A}}(\mathbf{\bar{r}}_{i})$ .

The Breit Hamiltonian is reduced to large components by standard techniques<sup>13,22</sup> to order  $(Z\alpha)^2$ Ry. The magnetic-field-dependent terms have been retained to order  $(Z\alpha)^2\mu_BH$  by Perl<sup>7</sup> and Abragam and Van Vleck.<sup>14</sup> The latter paper included the external magnetic field after the reduction to large components. However, the Hamiltonian is the same in both treatments.

The total Zeeman Hamiltonian  $\mathcal{K}_z$  contains seven terms:

$$\mathfrak{H}_{Z} = \sum_{i=0}^{n} \mathfrak{H}_{i} , \qquad (2.2)$$

$$\mathcal{H}_{0}' = \mu_{B} \vec{\mathbf{H}} \cdot (\vec{\mathbf{L}} + g_{S} \vec{\mathbf{S}}), \qquad (2.3)$$

$$\mathcal{H}_{1} = -\alpha^{2} \mu_{B} \vec{\mathbf{H}} \cdot \sum_{i} (\vec{\mathbf{l}}_{i} + 2\vec{\mathbf{s}}_{i}) T_{i} , \qquad (2.4)$$

$$\mathfrak{R}_{2} = \frac{1}{2} Z \, \alpha^{2} \mu_{B} \vec{\mathrm{H}} \cdot \sum_{i} \left[ \vec{\mathrm{s}}_{i} \times \vec{\nabla}_{i} (r_{i}^{-1}) \right] \times \vec{\mathrm{r}}_{i}, \qquad (2.5)$$

$$\mathscr{K}_{3} + \mathscr{K}_{4} = -\alpha^{2} \mu_{B} \vec{\mathrm{H}} \cdot \sum_{i < j} \left[ (\vec{s}_{i} + 2\vec{s}_{j}) \times \vec{\nabla}_{i} (r_{ij}^{-1}) \right] \times \vec{\mathrm{r}}_{i} ,$$
(2.6)

$$\mathscr{K}_{5} = -\alpha^{2} \mu_{B} \vec{\mathbf{H}} \cdot \sum_{i < j} \left[ r_{ij}^{-1} (\vec{\mathbf{r}}_{i} \times \vec{\mathbf{p}}_{j}) + r_{ij}^{-3} (\vec{\mathbf{r}}_{i} \times \vec{\mathbf{r}}_{j}) (\vec{\mathbf{r}}_{ij} \cdot \vec{\mathbf{p}}_{j}) \right],$$
(2.7)

$$\mathcal{K}_{6} = -(m/M) \mu_{B} \vec{H} \cdot \left[ \vec{L} + \sum_{i \neq j} \left( \vec{r}_{i} \times \vec{p}_{j} \right) \right].$$
(2.8)

The vector potential  $\vec{A}(\vec{r}_i)$  has been set equal to  $\frac{1}{2}\vec{H}\times\vec{r}_i$ .  $\mathcal{K}'_0$  is the lowest-order Zeeman effect. Here  $\vec{L}=\sum_i \vec{l}_i$  is the total orbital angular momentum and  $\vec{S}=\sum_i \vec{s}_i$  is the total spin.  $\mathcal{K}_1$  is analogous to the relativistic increase of mass and  $T_i$  is the kinetic energy of the *i*th electron. The reduction of the Breit equation (2.1) yields  $\mathcal{K}_2$ ,  $\mathcal{K}_3$ ,  $\mathcal{K}_4$ , and  $\mathcal{K}_5$ , which include terms analogous to spin-orbit, spin-other-orbit, and orbit-orbit interactions.<sup>14,15</sup> The last term in the Zeeman Hamiltonian  $\mathcal{K}'_6$  includes a correction for the motion of the center of mass,<sup>23</sup> where M is the atomic mass.

Radiative corrections are included by using the gyromagnetic ratio of the free electron<sup>24</sup>  $g_s$ :

$$\frac{1}{2}(g_{S}-2) = \alpha/2\pi - 0.328 \, 48 \, (\alpha/\pi)^{2} + (1.29 \pm 0.06) (\alpha/\pi)^{3}.$$
(2.9)

This is equivalent to the use of a Pauli Hamiltonian<sup>25</sup> that includes radiative effects.

#### **B.** Spherical-Tensor Notation

Innes and Ufford<sup>20</sup> recoupled the operators  $\mathcal{K}_i$ into spherical-tensor notation.<sup>21</sup> We define a tensor  $C_q^{(k)}$  that transforms as a spherical harmonic:

$$C_{q}^{(k)} = \left(\frac{4\pi}{2k+1}\right)^{1/2} Y_{kq}(\theta,\varphi).$$
 (2.10)

This is the qth component of a tensor of rank k.

We take the first term of  $\mathfrak{K}_6: -(m/M)\mu_B \vec{H} \cdot \vec{L}$ , define  $g_L = 1 - m/M$ , and rewrite  $\mathfrak{K}_0$  as

$$\mathcal{H}_{0} = \mu_{B} \vec{H} \cdot (g_{L} \vec{L} + g_{S} \vec{S}).$$
(2.11)

With the notation

$$\epsilon_{ij} = 1, \quad r_i < r_j$$
  
$$\epsilon_{ii} = 0, \quad r_i \ge r_i$$

the Zeeman Hamiltonian, in spherical-tensor notation, then becomes

$$\mathcal{H}_{o} = \mu_{B} \vec{\mathbf{H}} \cdot (g_{L} \vec{\mathbf{L}} + g_{S} \vec{\mathbf{S}}), \qquad (2.12)$$

$$\mathcal{H}_{1} = -\alpha^{2} \mu_{B} \vec{\mathbf{H}} \cdot \sum_{i} \left( \vec{\mathbf{l}}_{i} + 2\vec{\mathbf{s}}_{i} \right) T_{i} , \qquad (2.13)$$

$$\mathfrak{K}_{2} = \frac{2}{3} \alpha^{2} \mu_{B} \vec{H} \cdot \sum_{i} \frac{1}{\gamma_{i}} \left[ \vec{s}_{i} + (\frac{5}{2})^{1/2} \{ \vec{s}_{i} C_{i}^{(2)} \}^{(1)} \right], \quad (2.14)$$

$$\begin{aligned} \mathscr{K}_{3} + \mathscr{K}_{4} &= 2\alpha^{2}\mu_{B}\vec{H} \cdot \sum_{i \leq j} \left\{ \left(\vec{s}_{i} + 2\vec{s}_{j}\right) \sum_{k} (-1)^{k} (2k+1)^{1/2} \\ &\times \left[ \frac{1}{3} \left( k \frac{\epsilon_{ij}r_{i}^{k}}{r_{j}^{k+1}} - (k+1) \frac{\epsilon_{ji}r_{j}^{k}}{r_{i}^{k+1}} \right) \left\{ C_{i}^{(k)} C_{j}^{(k)} \right\}^{(0)} + \frac{\left[ k(k+1) \right]^{1/2}}{2\sqrt{6}} \left( \frac{\epsilon_{ij}r_{i}^{k}}{r_{j}^{k+1}} + \frac{\epsilon_{ji}r_{j}^{k}}{r_{i}^{k+1}} \right) \left\{ C_{i}^{(k)} C_{j}^{(k)} \right\}^{(1)} \\ &- \frac{\left[ k(k+1) \right]^{1/2}}{6\sqrt{2}} \left( \left( \frac{2k+3}{2k-1} \right)^{1/2} \frac{\epsilon_{ij}r_{i}^{k}}{r_{j}^{k+1}} - \left( \frac{2k-1}{2k+3} \right)^{1/2} \frac{\epsilon_{ji}r_{j}^{k}}{r_{i}^{k+1}} \right) \left\{ C_{i}^{(k)} C_{j}^{(k)} \right\}^{(2)} \\ &+ \frac{1}{2\sqrt{3}} \left( \frac{k(k-1)(2k-3)}{2k-1} \right)^{1/2} \frac{\epsilon_{ij}r_{i}^{k}}{r_{j}^{k+1}} \left\{ C_{i}^{(k-2)} C_{j}^{(k)} \right\}^{(2)} \\ &- \frac{1}{2\sqrt{3}} \left( \frac{(k+1)(k+2)(2k+5)}{2k+3} \right)^{1/2} \frac{\epsilon_{ji}r_{j}^{k}}{r_{i}^{k+1}} \left\{ C_{i}^{(k+2)} C_{j}^{(k)} \right\}^{(2)} \right] \right\}^{(1)} , \end{aligned}$$

$$(2.15)$$

$$\begin{split} \mathfrak{K}_{5} &= \frac{1}{\sqrt{3}} \; \alpha^{2} \mu_{B} \overrightarrow{\mathbf{H}} \cdot \sum_{i < j} \sum_{k} (-1)^{k} \left\{ \left( \frac{\epsilon_{ji} r_{i}^{k}}{r_{i}^{k+1}} + \frac{\epsilon_{ij} r_{i}^{k+2}}{r_{j}^{k+3}} \right) \\ &\times \left( \frac{k(k+3)}{2k+3} \left[ (2k+1)^{1/2} \left\{ C_{i}^{(k)} \left\{ C_{j}^{(k)} \overrightarrow{\mathbf{1}}_{j} \right\}^{(1)} - (2k+5)^{1/2} \left\{ C_{i}^{(k+2)} \left\{ C_{j}^{(k+2)} \overrightarrow{\mathbf{1}}_{j} \right\}^{(k+2)} \right\}^{(1)} \right] \right. \\ &\left. - 2 \left( \frac{2k+1}{2k+3} \right)^{1/2} \left[ (2k+1)^{1/2} \left\{ C_{i}^{(k)} \left\{ C_{j}^{(k)} \overrightarrow{\mathbf{1}}_{j} \right\}^{(k+1)} \right\}^{(1)} \right. \\ &\left. + \left( \frac{(k+1)(2k+5)}{k+2} \right)^{1/2} \left\{ C_{i}^{(k+2)} \left\{ C_{j}^{(k)} \overrightarrow{\mathbf{1}}_{j} \right\}^{(k+1)} \right\}^{(1)} \right] \right) \right. \\ &\left. + \left( (k+3) \frac{\epsilon_{ij} r_{i}^{k+2} \partial r_{j}}{r_{j}^{k+2}} - k \frac{\epsilon_{ji} r_{j}^{k+1} \partial r_{j}}{r_{i}^{k+1}} \right) \frac{1}{2k+3} \right. \\ &\left. \times \left[ \left[ k(k+1)(2k+1) \right]^{1/2} \left\{ C_{i}^{(k)} C_{j}^{(k)} \right\}^{(1)} - \left[ (k+2)(k+3)(2k+5) \right]^{1/2} \left\{ C_{i}^{(k+2)} C_{j}^{(k+2)} \right\}^{(1)} \right) \right\}, \end{split}$$

$$\mathfrak{K}_{6} = -2(m/M)\,\mu_{B}\vec{\mathrm{H}} \cdot \sum_{i < j} \left[ 2(r_{i}/r_{j}) \left\{ C_{i}^{(1)} \left\{ C_{j}^{(1)} \vec{\mathrm{I}}_{j} \right\}^{(1)} \right\}^{(1)} - \sqrt{2} \, r_{i} \, \partial r_{j} \left\{ C_{i}^{(1)} \, C_{j}^{(1)} \right\}^{(1)} \right].$$
(2.17)

The subscripts on the spherical tensors and spin operators in these equations refer to the electron and not to the component of the tensor.

The calculation of the Zeeman effect requires the use of a specific wave function. In Sec. III the approximations used for the helium wave function are discussed.

## **III. HELIUM WAVE FUNCTIONS**

The Schrödinger equation for helium has not been solved exactly, but both analytic and numerical approximations for the helium wave function have been used. Series expansions in a Hylleraas basis<sup>26,27</sup> have been used to approximate the helium eigenvalues and eigenfunctions. Bartlett<sup>28</sup> and Gronwall<sup>29</sup> demonstrated that these expansions do not solve the Schrödinger equation for helium even in the limit of an infinite number of terms. However, such series do give excellent approximations to the eigenvalue if a sufficient number of terms is used. Fock<sup>30</sup> developed a series solution for helium using logarithmic terms. The Hylleraas-like solutions are sufficiently accurate for the calculation of the Zeeman effect.

#### A. Numerical Wave Functions for 2<sup>3</sup>P Helium

The wave function  $\Psi_0$ , which is the solution of  $H_0\Psi_0 = E_0\Psi_0$ , is to be approximated.  $H_0$  is the Schrödinger Hamiltonian for helium in atomic units:

$$H_0 = -\frac{1}{2} \nabla_1^2 - \frac{1}{2} \nabla_2^2 - 2/r_1 - 2/r_2 + 1/r_{12}.$$
(3.1)

The spatial part of the  $2 {}^{3}P_{J}$  wave function is antisymmetric with respect to the interchange of electron coordinates. Our standard Hylleraas basis is taken as<sup>16</sup>

$$U_{lmn}(1,2) = \frac{1-P_{12}}{4\pi\sqrt{2}} \tilde{r}_{1} r_{1}^{m} r_{2}^{n} r_{12}^{l}$$

$$\times e^{-(\kappa\sigma/2)r_{1}} e^{-(\kappa/2)r_{2}}.$$
(3.2)

 $P_{12}$  is an operator that interchanges coordinates  $r_1$  and  $r_2$ . The screening parameters  $\kappa$  and  $\sigma$  are determined by a variational calculation. The integers l, m, n are non-negative  $l \ge 0$ ,  $m \ge 0$ ,

 $n \ge 0$ . The wave function is a series in  $U_{lmn}$ :

$$\Psi_{0} = \sum_{l,m,n=0}^{l+m+n\leq\omega} C_{lmn} U_{lmn}(1,2), \qquad (3.3)$$

where the coefficients  $C_{Imn}$  and the energy are determined from the variational principle:

$$\delta\langle \Psi_0 | H_0 - E_0 | \Psi_0 \rangle = 0. \tag{3.4}$$

The interelectron distance is

$$\begin{aligned} r_{12} &= |\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2| \\ &= (r_1^2 + r_2^2 - 2r, r_2 \cos \theta_{12})^{1/2}, \end{aligned} \tag{3.5}$$

where  $\theta_{12}$  is the angle between  $\vec{r}_1$  and  $\vec{r}_2$ .

The basis  $U_{lmn}$  has the symmetry of a (sp) configuration:

$$\Psi = (1/\sqrt{2}) \left[ \phi_{1s}(r_1) \Psi_{2p}(r_2) - \Psi_{1s}(r_1) \phi_{2p}(r_2) \right] \quad (3.6)$$

when correlation is neglected. The single-particle wave functions are taken as hydrogenic in the

TABLE I. Ordering of terms in Hylleraas basis.

N	l	m	n	ω
1	0	0	0	0
2	0	0	1	1
3	0	1	0	1
4	1	0	0	1
5	0	0	2	2
6	0	1	1	2
7	0	2	0	2
8	1	0	1	2
9	1	1	0	2
10	2	0	0	2
11	0	0	3	3
12	0	1	2	3
13	0	2	1	3
14	0	3	0	3
15	1	0	2	3
16	1	1	1	3
17	1	2	0	3
18	2	0	1	3
19	2	1	0	3
20	3	0	0	3
21	0	0	4	4
22	0	1	3	4
23	0	2	2	4
24	0	3	1	4
25	0	4	0	4
26	1	0	3	4
27	1	1	2	4
28	1	2	1	4
29	1	3	0	4
30	2	0	2	4
31	2	1	1	4
32	2	2	0	4
33	3	0	1	4
34	3	1	0	4
35	4	0	0	4

lowest-order approximation.

We have calculated wave functions for the index  $\omega$  in Eq. (3.3) from one through eight. The total number of terms in a wave function for a given  $\omega$  is

$$N=\frac{1}{6}(\omega+1)(\omega+2)(\omega+3).$$

Thus wave functions with 4, 10, 20, 35, 56, 84, 120, and 165 terms were computed. In addition, a single-term and a two-term wave function were calculated. Table I presents the ordering of the variables l, m, and n for  $\omega \leq 4$ .

We have used the screening parameters  $\kappa$  and  $\sigma$  given by Schwartz<sup>16</sup>:

$$\kappa = 4.61999994516372$$
 (3.7)

$$\sigma = 0.289\,999\,999\,105\,930. \tag{3.8}$$

These values may be compared to the results in an early calculation by Eckart<sup>31</sup> and reported in a different form:

$$\kappa_E = 3.98, \tag{3.9}$$

$$\sigma_E = 0.27.$$
 (3.10)

The energy eigenvalue of  $2^{3}P$  helium obtained from our variational calculation is presented in Table II. The extrapolated energy is in excellent agreement with Schwartz's best result<sup>16</sup> of -2.1331641908 a.u. These wave functions were calculated in double precision on an IBM 360/67 machine.

#### **B.** Integrals

Many integrals<sup>32</sup> are needed to calculate the matrix elements of  $\mathcal{K}_i$  with  $\Psi_0$  in Eq. (3.3). The major ones are

$$A(L, M, N) = \int \frac{d\tau_1}{4\pi} \int \frac{d\tau_2}{4\pi} e^{-ar_1} e^{-br_2} \times r_1^{M-2} r_2^{N-2} r_{12}^{L-2}, \qquad (3.11)$$

TABLE II.  $2^{3}P$  energy eigenvalues.

N	Energy (a.u.)
1	-2.072 137 762
2	-2.123103128
4	-2.129471788
10	-2.132678402
20	-2.133 085 039
35	-2.133140222
56	-2.133157595
84	-2.133162287
120	-2.133163594
165	-2.133163981
Extrapolated	-2.1331642

$$B(L, M, N) = \int \frac{d\tau_1}{4\pi} \int \frac{d\tau_2}{4\pi} e^{-ar_1} e^{-br_2} \times r_1^{M-2} r_2^{N-2} r_{12}^{L-2} \cos\theta_{12}.$$
(3.12)

There are two types of A and B integrals.  $A_d(L, M, N)$  and  $B_d(L, M, N)$  are the direct integrals with  $a = \kappa \sigma$ ,  $b = \kappa$ .  $A_e(L, M, N)$  and  $B_e(L, M, N)$  are the exchange integrals with  $a = b = \frac{1}{2}\kappa(1 + \sigma)$ . The computer calculates these integrals by the use of recursion relations:

$$A(L, M, N) = A(L - 2, M + 2, N) + A(L - 2, M, N + 2)$$
$$-2B(L - 2, M + 1, N + 1)$$
(3.13)

and

$$B(L, M, N) = \frac{L-2}{L+2} \left[ B(L-2, M+2, N) + B(L-2, M, N+2) -2A(L-2, M+1, N+1) \right].$$
(3.14)

These relations may be obtained with

$$r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_{12} \tag{3.15}$$

and

$$\int \frac{d\Omega_{1}}{4\pi} \int \frac{d\Omega_{2}}{4\pi} (\sin^{2}\theta_{12}) r_{12}^{L} = -\frac{2}{L+2} \int \frac{d\Omega_{1}}{4\pi} \int \frac{d\Omega_{2}}{4\pi} \times (\cos\theta_{12}) \frac{r_{12}^{L+2}}{r_{1}r_{2}}.$$
(3.16)

If we define

$$F(M, N; \alpha, \beta) = \int_0^\infty dr \ e^{-\alpha r} \ r^{M-1} \int_r^\infty ds \ e^{-\beta s} s^{N-1},$$
(3.17)

then we may show

$$A(2, M, N) = \frac{M!N!}{a^{M+1}b^{N+1}}, \qquad (3.18)$$

$$B(2, M, N) = 0,$$
 (3.19)

$$A(1, M, N) = F(M+1, N; a, b) + F(N+1, M; b, a),$$
(3.20)

$$B(1, M, N) = \frac{1}{3} \left[ F(M+2, N-1; a, b) + F(N+2, M-1; b, a) \right].$$
(3.21)

The F integrals are calculated using

$$F(M, 1; \alpha, \beta) = \frac{1}{\beta} \frac{(M-1)!}{(\alpha+\beta)^{M}},$$
 (3.22)

$$F(M, N; \alpha, \beta) = \frac{(M+N-2)!}{\beta (\alpha+\beta)^{M+N-1}} + \frac{N-1}{\beta} F(M, N-1; \alpha, \beta).$$
(3.23)

The recursion relations above are valid for A integrals with  $L \ge 1$ ,  $M \ge 1$ ,  $N \ge 1$ , and for B integrals with  $L \ge 1$ ,  $M \ge 2$ ,  $N \ge 2$ .

In the Appendix the general expansion of  $r_{12}^n$ in terms of Legendre polynomials as given by Sack<sup>33</sup> is discussed.

The lowest-order term in the expansion

$$r_{12}^{-2} = \frac{1}{2r_1r_2} \ln \frac{(r_1 + r_2)}{|r_1 - r_2|} + \cdots$$
(3.24)

is needed in the A and B integrals when L = 0. Thus

$$A_{d}(0, M, N) = \frac{1}{2} \left[ F_{la}(M, N) + F_{lb}(N, M) \right], \qquad (3.25)$$

$$A_{e}(0, M, N) = \frac{1}{2} \left[ F_{lc}(M, N) + F_{lc}(N, M) \right]; \qquad (3.26)$$

$$B_{d}(0, M, N) = \frac{1}{4} [F_{Ia}(M+1, N-1) + F_{Ia}(M-1, N+1)] + F_{Ib}(N+1, M-1) + F_{Ib}(N-1, M+1)] - \frac{1}{2} [F(M, N; \kappa\sigma, \kappa) + F(N, M, \kappa, \kappa\sigma)],$$
(3.27)

$$B_{e}(0, M, N) = \frac{1}{4} \left[ F_{lc}(M+1, N-1) + F_{lc}(M-1, N+1) + F_{lc}(N+1, M-1) + F_{lc}(N-1, M+1) \right] \\ - \frac{1}{2} \left[ F(M, N; \delta, \delta) + F(N, M; \delta, \delta) \right],$$
(3.28)

where  $\delta = \frac{1}{2}\kappa(1 + \sigma)$ . The  $F_l$  integrals are

$$F_{I}(M,N; \alpha,\beta) = \int_{0}^{\infty} dr \ e^{-\alpha r} \ r^{M-1}$$
$$\times \int_{r}^{\infty} ds \ e^{-\beta s} \ s^{N-1} \ln \frac{s+r}{s-r} , \quad (3.29)$$

and

$$\begin{aligned} F_{la}(M,N) &= F_l(M,N; \ \kappa\sigma, \kappa), \\ F_{lb}(M,N) &= F_l(M,N; \ \kappa, \kappa\sigma), \\ F_{lc}(M,N) &= F_l(M,N; \ \delta, \delta). \end{aligned} \tag{3.30}$$

The  $F_i$  integrals may be written as sums of products of various functions.<sup>32</sup>

For the A and B integrals with M=0,  $N \ge 1$  or  $M \ge 1$ , N=0 when  $L \ge 1$ , we need  $F(M, N; \alpha, \beta)$  for N=0 and N=-1:

$$F(M, -N; \alpha, \beta) = \frac{(M-N-1)!}{N(\alpha+\beta)^{M-N}}$$
$$-\frac{\beta}{N} F(M, -N+1; \alpha, \beta). \quad (3.31)$$

Equation (3.31) can be obtained by partial integration. The value of  $F(M, 0; \alpha, \beta)$  was not calculated with a forward recursion method because of loss of accuracy by subtraction. Rather, a backward recursion relation is used:

$$F(M-1,0;\alpha,\beta) = \frac{1}{M-1} \times \left(\frac{(M-2)!}{(\alpha+\beta)^{M-1}} + \alpha F(M,0;\alpha,\beta)\right).$$
(3.32)

F is approximated for a large value of M, and then Eq. (3.32) is used.

## C. Numerical Wave Function for $2^{3}S_{1}$ Helium

A Hylleraas-like numerical wave function has been evaluated for the  $2^{3}S_{1}$  state of helium. The form of the wave function<sup>16,34</sup> is

$$\Psi = \left(\frac{1-P_{12}}{(8\pi)^{1/2}}\right) \sum_{L,M,N} D_{LMN} v_{LMN}(1,2), \qquad (3.33)$$

where  $P_{12}$  exchanges operator subscripts, the  $D_{LMN}$  are coefficients to be evaluated, and

$$v_{LMN}(1,2) = (1 - \frac{1}{2}Z_b r_2) e^{-(Z_a/2)r_1} \\ \times e^{-(Z_b/2)r_2} r_1^M r_2^N r_{12}^L.$$

For a preliminary 35-term wave function we obtained E = -2.175212 a.u., which is in adequate agreement with the result of Pekeris<sup>35</sup> of E = -2.175229 a.u. with 715 terms.

The best result for the convergence of the energy eigenvalue was obtained with the screening factors  $Z_a = 4.25$  and  $Z_b = 1.66$ . These factors differ from the results of Traub and Foley,<sup>36</sup> who obtained  $Z_a = 4.12$  and  $Z_b = 1.20$ .

#### IV. RESULTS AND DISCUSSION

## A. Hydrogenic Approximation for $2^{3}P$ Helium

We approximate the helium wave function with a product of 1s and 2p hydrogenic wave functions and calculate the Zeeman effect.<sup>12</sup>

The wave function is taken as an (sp) configuration

$$\Psi' = (1/\sqrt{2}) [R_{1s}(r_1) R_{2p}(r_2) - R_{1s}(r_2) R_{2p}(r_1)] \chi \Omega, \qquad (4.1)$$

where  $\chi$  includes spin variables,  $\Omega$  includes the angular variables,

$$R_{1s}(r_i) = R_{10}(r_i)$$
$$= 2Z_1^{3/2} e^{-Z_1 r_i},$$

and

$$R_{2p}(r_i) = R_{21}(r_i)$$
  
=  $(Z_2^{5/2}/2\sqrt{6})r_i e^{-(Z_2/2)r_i}$ .

The values of the screening constants are  $Z_1 = 1.99$ ,  $Z_2 = 1.09$ .<sup>31</sup>  $Z_1$  and  $Z_2$  are related to  $\kappa$  and  $\sigma$  in Eq. (3.2):

$$\begin{aligned} \kappa &= 2Z_1 = 3.98, \\ \sigma &= Z_2/2Z_1 = 0.27. \end{aligned} \tag{4.3}$$

Matrix elements of the Zeeman Hamiltonian  $\mathcal{K}_Z$ in Eqs. (2.12)-(2.17) using the Russell-Saunders eigenstate  $|{}^{3}P_J m_J \rangle$  are calculated. The result  $\langle {}^{3}P_J m_J | \mathcal{K}_Z | {}^{3}P_J, m_J \rangle$  is given in terms of radial integrals  $R_i$  and various n-j symbols:

$$\langle |\mathcal{K}_{0}| \rangle = \sqrt{6} \ \mu_{B} H(-1)^{1-m_{J}} (2J+1)^{1/2} (2J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix} \begin{cases} J & 1 & J' \\ 1 & 1 & 1 \end{cases} \begin{bmatrix} (-1)^{J+J'} g_{L} + g_{S} \end{bmatrix},$$
(4.4)

$$\langle |\mathcal{H}_{1}| \rangle = -\sqrt{6} \ \alpha^{2} \mu_{B} H (-1)^{1-m_{J}} (2J+1)^{1/2} (2J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix} \begin{cases} J & 1 & J' \\ 1 & 1 & 1 \end{cases} \{ R_{1} + [1 + (-1)^{J+J'}] R_{2} \},$$
 (4.5)

$$\langle |3\mathcal{C}_{2}| \rangle = \sqrt{6} \ \alpha^{2} \mu_{B} H(-1)^{1-m} J(2J+1)^{1/2} (2J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix}$$

$$\times \left( \frac{1}{3} \begin{cases} J & 1 & J' \\ 1 & 1 & 1 \end{cases} (R_{3} + R_{4}) + (-1)^{J} \begin{cases} 1 & 1 & 2 \\ 1 & 1 & 1 \\ J & J' & 1 \end{cases} R_{4} \right),$$

$$(4.6)$$

$$\langle |\mathcal{3C}_{3} + \mathcal{3C}_{4}| \rangle = \sqrt{6} \ \alpha^{2} \mu_{B} H(-1)^{J-m_{J}} (2 J+1)^{1/2} (2 J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix}$$

$$\times \left( \begin{cases} 1 & 1 & 2 \\ 1 & 1 & 1 \\ J & J' & 1 \end{cases} \left. \begin{pmatrix} 3_{2}R_{6} + 2R_{7} - \frac{3}{2}R_{8} \end{pmatrix} + \begin{cases} 1 & 1 & 0 \\ 1 & 1 & 1 \\ J & J' & 1 \end{cases} \left. \begin{pmatrix} R_{7} - \frac{3}{2}R_{6} - \frac{3}{2}R_{5} \end{pmatrix} \right),$$

$$(4.7)$$

$$\langle |\mathcal{K}_{5}| \rangle = \sqrt{6} \ \alpha^{2} \mu_{B} H (-1)^{J+J'+1-m_{J}} (2J+1)^{1/2} (2J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix}$$

$$\times \begin{cases} J & 1 & J' \\ 1 & 1 & 1 \end{cases} \ (-\frac{1}{3}R_{5} + \frac{2}{15}R_{7} - \frac{1}{3}R_{8} + \frac{2}{15}R_{9} + \frac{1}{30}R_{10} - \frac{1}{30}R_{11} - \frac{2}{15}R_{12} + \frac{2}{15}R_{13}),$$

$$(4.8)$$

(4.2)

$$\langle |\mathcal{K}_{6}|\rangle = \sqrt{6} \ \mu_{B}H(m/M)(-1)^{1-m_{J}+J+J'}(2J+1)^{1/2}(2J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix} \begin{pmatrix} J & 1 & J' \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{3}R_{16} - \frac{1}{3}R_{17} + \frac{2}{3}R_{18} \end{pmatrix}.$$
(4.9)

The radial integrals are defined as either direct D or exchange E integrals. A direct integral is of the form

 $\int R_{1s}(r_i) R_{2p}(r_j) \mathcal{K}_Z R_{1s}(r_i) R_{2p}(r_j) d\tau,$ and an exchange integral is of the form

$$\int R_{1s}(r_i)R_{2p}(r_j)\mathcal{K}_{Z}R_{1s}(r_j)R_{2p}(r_i)d\tau.$$

The subscript sp indicates  $r_i = r_1$  and  $r_j = r_2$ ; ps is the reverse. The radial integrals in the matrix elements of the Zeeman Hamiltonian are

$$\begin{split} R_{1} &= \langle |T_{1}| \rangle_{B_{sp}} = 1.98, \quad R_{2} = \langle |T_{1}| \rangle_{F_{ps}} = 0.149, \quad R_{3} = \left\langle \left| \frac{1}{r_{1}} \right| \right\rangle_{B_{sp}} = 1.99, \\ R_{4} &= \left\langle \left| \frac{1}{r_{1}} \right| \right\rangle_{D_{ps}} = 0.273, \quad R_{5} = \left\langle \left| \frac{1}{r_{1}} \right| \right\rangle_{F_{sp}} (r_{2} \leq r_{1}) = 0.0046, \\ R_{6} &= \left\langle \left| \frac{1}{r_{1}} \right| \right\rangle_{D_{ps}} (r_{2} \leq r_{1}) = 0.267, \quad R_{7} = \left\langle \left| \frac{r_{1}}{r_{2}^{2}} \right| \right\rangle_{E} (r_{1} \leq r_{2}) = 0.0079, \\ R_{8} &= \left\langle \left| \frac{r_{1}^{2}}{r_{2}^{3}} \right| \right\rangle_{D_{sp}} (r_{1} \leq r_{2}) = 0.025, \quad R_{9} = \left\langle \left| \frac{r_{1}^{3}}{r_{2}^{4}} \right| \right\rangle_{E} (r_{1} \leq r_{2}) = 0.0043, \\ R_{10} &= \left\langle \left| \frac{r_{2}^{2} \partial r_{2}}{r_{1}^{2}} \right| \right\rangle_{E_{ps}} (r_{2} \leq r_{1}) = 0.003, \quad R_{11} = \left\langle \left| \frac{r_{2}^{2} \partial r_{2}}{r_{1}^{2}} \right| \right\rangle_{E_{sp}} (r_{2} \leq r_{1}) = -0.0177, \\ R_{12} &= \left\langle \left| \frac{r_{1}^{3} \partial r_{2}}{r_{2}^{3}} \right| \right\rangle_{E_{ps}} (r_{1} \leq r_{2}) = 0.0007, \quad R_{13} = \left\langle \left| \frac{r_{1}^{3} \partial r_{2}}{r_{2}^{3}} \right| \right\rangle_{E_{sp}} (r_{1} \leq r_{2}) = -0.0133, \\ R_{14} &= \left\langle |r_{1}^{2}| \right\rangle_{E_{sp}} = 0.758, \quad R_{15} = \left\langle |r_{1}^{2}| \right\rangle_{D_{sp}} = 25.25, \quad R_{16} = \left\langle |r_{1} \partial r_{2}| \right\rangle_{E_{ps}} = 0.020, \\ R_{17} &= \left\langle |r_{1} \partial r_{2}| \right\rangle_{E_{sp}} = -0.1339, \quad R_{18} = \left\langle \left| \frac{r_{1}}{r_{2}} \right| \right\rangle_{E} = 0.0569. \end{split}$$

## These radial integrals differ slightly from the previous calculation.<sup>12, 37</sup>

The g factors are defined by the following grouping of the matrix elements of the Zeeman Hamiltonian:

$$\langle Jm_{J} | \Im C_{Z} | J'm_{J} \rangle = (-1)^{1-m_{J}} (2J+1)^{1/2} (2J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix} \sqrt{6} \\ \times \left[ \begin{cases} J & 1 & J' \\ 1 & 1 & 1 \end{cases} [g'_{S} + (-1)^{J+J'}g'_{L}] + \begin{cases} 1 & 1 & 2 \\ 1 & 1 & 1 \\ J & J' & 1 \end{cases} (-1)^{J}g_{X} \right] \mu_{B}H,$$

$$(4.10)$$

where

$$g'_{L} = g_{L} + \alpha^{2} (-R_{2} - \frac{1}{3}R_{5} + \frac{2}{15}R_{7} - \frac{1}{3}R_{8} + \frac{2}{15}R_{9} + \frac{1}{30}R_{10} - \frac{1}{30}R_{11} - \frac{2}{15}R_{12} + \frac{2}{15}R_{13}) + (m/M)(\frac{1}{3}R_{16} - \frac{1}{3}R_{17} + \frac{2}{3}R_{18});$$

$$g'_{S} = g_{S} + \alpha^{2}(-R_{1} - R_{2} + \frac{1}{3}R_{3} + \frac{1}{3}R_{4} - \frac{1}{2}R_{5} - \frac{1}{2}R_{6} + \frac{1}{3}R_{7});$$

$$g_{X} = \alpha^{2}(R_{4} - \frac{3}{2}R_{6} - 2R_{7} + \frac{3}{2}R_{8}). \qquad (4.11)$$

The g factor  $g_{\chi}$ , of order  $\alpha^2$ , comes from the matrix elements of a tensor composed of a spin vector and a spherical tensor of rank 2 such as  $\{\mathbf{\bar{sC}}^{(2)}\}^{(1)}$ , which arises from the recoupling of

the reduced Breit Hamiltonian in spherical tensors.  $g_x$  vanishes in S states.

The g factors can be evaluated to give theoretical values in the hydrogenic approximation

$$g'_{S} = g_{S} - 80.3 \times 10^{-6},$$
  
 $g'_{L} = g_{L} + 3.8 \times 10^{-6},$  (4.12)  
 $g_{X} = -5.6 \times 10^{-6}.$ 

This result may be compared to the hydrogenic approximation<sup>12</sup> using less precise radial integrals

$$g'_{S} = g_{S} - (79.9 \pm 3.5) \times 10^{-6},$$
  

$$g'_{L} = g_{L} + (1.1 \pm 1.5) \times 10^{-6},$$
  

$$g_{X} = (-3.2 \pm 4.4) \times 10^{-6}.$$

## B. Matrix Elements Using the Numerical Wave Function for 2<sup>3</sup>P Helium

Once the integrals in Sec. III B are computed, the calculation of the matrix elements of the Zeeman Hamiltonian for the  $2^{3}P$  state is straightforward.  $\mathcal{X}_{0}$  has no radial or angular parts; hence we obtain the same result as Eq. (4.4):

If we let  $\Re_{Z} = \sum_{i=0}^{6} \Re_{i}$ , we may write the matrix elements of the complete Zeeman Hamiltonian:

We note that the matrix elements of the Zeeman Hamiltonian, using the numerical wave function Eq. (3.3), is of the same form as Eq. (4.10) where the pure (sp) configuration is assumed. Owing to the presence of correlation in the Hylleraas basis, one can consider the basis to include excited configurations as well as the (sp) configuration—but this does not change the Zeeman Hamiltonian matrix.<sup>12</sup>

A computer calculation is performed to evaluate the radial integrals. Table III gives the value of the g factors for each of the ten wave functions. The series of ten values for each g factor is extrapolated by standard techniques.<sup>32</sup> Essentially

TABLE III.  $2^{3}P_{J}$  helium g factors using numerical wave functions.

Terms	$(g'_S - g_S) \times 10^6$	$(g_L' - g_L)  imes 10^6$	$g_X \times 10^6$
1	-115.739	3.942	-6.74
2	-85.300	10.418	-6.38
4	-82.953	7.948	-5.59
10	-80.676	8,533	-4.99
20	-80.453	9.379	-4.68
35	-80.457	9.917	-4.64
56	-80.460	10.337	-4.54
84	-80.462	10.879	-2.25
120	-80.462	11.070	-0.57
165	-80.462	10.782	-3.47
Extrapolated	$-80.46 \pm 0.01$	$10.6 \pm 0.4$	$-3.5 \pm 2.5$

the g factors are considered a function of the index  $\omega$ , which is extrapolated to infinity. The accuracy of a calculation of this type is difficult to assess. The calculation was performed in double precision to help eliminate loss of accuracy by subtraction. The error limits on the extrapolated values in Table III are based on the convergence of the g factors as  $\omega$  is increased.

We can compare the result of this calculation with the hydrogenic approximations given in Eq. (4.12) and the experimentally determined values.<sup>12</sup> The comparison of the experimental and theoretical g factors appears in Table IV. There is good agreement between the experimental and extrapolated values reported here. The calculated values of  $g'_L$  and  $g_x$  are both within one standard deviation of the experimental error. The theoretical value of  $g'_{s}$  calculated with the numerical wave function agrees well with the hydrogenic approximation and agrees with experiment within two standard deviations of the experimental error. Because of the small discrepancy between the experimental and theoretical values of  $g'_{s}$ , a more accurate measurement of the Zeeman effect in  $2^{3}P_{J}$  helium would be useful. The measurement of the g factors in  $2^{3}P$  helium<sup>12</sup> is important for the determination of the  $2{}^{3}P_{1}-2{}^{3}P_{2}$  and  $2{}^{3}P_{1}-2{}^{3}P_{0}$  fine-structure intervals.<sup>1, 12</sup>

The  $2^{1}P_{1}$  state of helium lies  $6 \times 10^{4}$  GHz above the  $2^{3}P_{J}$  states. Spin-orbit interaction between states of the same total angular momentum Jleads to a partial breakdown of L-S coupling. Araki<sup>38</sup> and Pekeris<sup>39</sup> have shown that the singlet admixture shifts the energy of the  $2^{3}P_{1}$  state by about 4.5 MHz. Second-order perturbations from the singlet state do not contribute because the Hamiltonian  $\mathcal{K}_{Z}$  is diagonal in L and S. Hence the lowest-order contributions to the Zeeman effect are third-order perturbations of the form

TABLE IV. Comparison of g factors in  $2^{3}P_{J}$  helium.

(g's - )	g <sub>S</sub> )×10 <sup>6</sup>
Extrapolated	$-80.46 \pm 0.01$
Hydrogenic	-80.3
Experiment	$-76.0 \pm 2.4$
$(g_t' - )$	$(g_r) \times 10^6$
Extrapolated	$10.6 \pm 0.4$
Hydrogenic	3.8
Experiment	$3.8 \pm 9.0$
	~ 106
g <sub>x</sub>	× 10°
Extrapolated	$-3.5 \pm 2.5$
Hydrogenic	-5.6
Experiment	$4.0 \pm 25.0$

$$\frac{\langle {}^{3}P_{1}|\text{spin-orbit}|{}^{1}P_{1}\rangle\langle {}^{1}P_{1}|\mathscr{C}_{Z}|{}^{1}P_{1}\rangle\langle {}^{1}P_{1}|\text{spin-orbit}|{}^{3}P_{1}\rangle}{[E(2 {}^{3}P_{1}) - E(2 {}^{1}P_{1})]^{2}}.$$
(4.15)

The magnitude of this perturbation is approximately  $10^{-7}$  GHz for magnetic fields of several kG and hence would change the g factors by less than 0.1 ppm.

# C. Relativistic Contributions to the Magnetic Moment of $2^{3}S_{1}$ Helium

Perl and Hughes<sup>6</sup> evaluated the relativistic contributions to the magnetic moment of  $2^{3}S_{1}$  helium. Drake *et al.*<sup>18</sup> measured the ratio of the atomic  $g_{J}$  value of  $2^{3}S_{1}$  helium to that of  $1^{2}S_{1/2}$  hydrogen by means of an atomic beam magnetic resonance method to obtain the ratio

$$\frac{g_{J}(\text{He}, 2^{3}\text{S}_{1})}{g_{J}(\text{H}, 1^{2}\text{S}_{1/2})} \bigg|_{\text{expt}} = 1 - (23.3 \pm 0.8) \times 10^{-6}. \quad (4.16)$$

The theoretical ratio is<sup>6</sup>

$$\frac{g_J(\text{He}, 2^{3}S_1)}{g_J(\text{H}, 1^{2}S_{1/2})}\Big|_{\text{theory}} = 1 - (23.3 \pm 1.0) \times 10^{-6}.$$
(4.17)

The Zeeman Hamiltonian in Eqs. (2.12)-(2.17) can be used to find the g factor of the  $2^{3}S_{1}$  state of helium.

Matrix elements of the Zeeman Hamiltonian yield

$$({}^{3}S_{1}| \mathcal{H}_{0}| {}^{3}S_{1}) = \mu_{B}Hg_{S}, \qquad (4.18)$$

$$({}^{3}S_{1}|{}^{3}C_{1}|{}^{3}S_{1}) = -\alpha^{2}\mu_{B}H\langle T\rangle, \qquad (4.19)$$

$$({}^{3}\mathrm{S}_{1}|\mathcal{H}_{2}|{}^{3}\mathrm{S}_{1}) = \frac{1}{3}\alpha^{2}\mu_{B}H\left(\left\langle\frac{1}{r_{1}}\right\rangle + \left\langle\frac{1}{r_{2}}\right\rangle\right), \qquad (4.20)$$

$$({}^{3}S_{1}|\mathcal{H}_{3} + \mathcal{H}_{4}|{}^{3}S_{1}) = -\frac{1}{2}\alpha^{2}\mu_{B}H\left\langle\frac{1}{r_{12}}\right\rangle,$$
 (4.21)

$$({}^{3}S_{1}|\mathcal{K}_{5}|{}^{3}S_{1}) = 0,$$
 (4.22)

$$({}^{3}S_{1}|\mathcal{H}_{6}|{}^{3}S_{1}) = 0,$$
 (4.23)

where  $T = T_1 + T_2$  is the total kinetic energy of both electrons. The matrix elements of the total Hamiltonian  $\Re_z = \sum_{i=0}^6 \Re_i$  may be written

$$({}^{3}S_{1}|\mathcal{K}_{Z}|{}^{3}S_{1}) = \mu_{B}H\left[g_{S} + \alpha^{2}\left(\frac{1}{3}\left\langle\frac{1}{r_{1}}\right\rangle + \frac{1}{3}\left\langle\frac{1}{r_{2}}\right\rangle - \langle T \rangle - \frac{1}{2}\left\langle\frac{1}{r_{12}}\right\rangle\right)\right].$$

$$(4.24)$$

By the use of the virial theorem,<sup>19</sup> one can establish

$$\left\langle \frac{1}{r_1} \right\rangle + \left\langle \frac{1}{r_2} \right\rangle = \langle T \rangle + \frac{1}{2} \left\langle \frac{1}{r_{12}} \right\rangle.$$
 (4.25)

Hence

$$({}^{3}S_{1}|\mathscr{K}_{Z}|{}^{3}S_{1}) = \mu_{B}Hg'_{S}, \qquad (4.26)$$

where

$$g'_{s} = g_{s} - 2\alpha^{2} \left( \frac{1}{3} \langle T \rangle + \frac{1}{6} \left\langle \frac{1}{r_{12}} \right\rangle \right).$$

$$(4.27)$$

This result agrees exactly with the calculation of Perl and Hughes.<sup>6</sup> Pekeris<sup>35</sup> has calculated the value of the matrix elements of T and  $r_{12}^{-1}$  using a wave function with 715 terms:

$$\langle T \rangle = 2.175\ 229\ 378\ 24,$$
 (4.28)

$$\left\langle \frac{1}{r_{12}} \right\rangle = 0.268\,197\,855\,3.$$
 (4.29)

Hence, using Eq. (4.27), the value for  $g'_s$  is

$$g'_{\rm S} = g_{\rm S} - 81.98322 \times 10^{-6}.$$
 (4.30)

This result is also in excellent agreement with Perl and Hughes. Thus, to order  $\alpha^2$ , we may write

$$g_J(\text{He}, 2^{3}\text{S}_1) = g_S(1 - 40.99161 \times 10^{-6}),$$
 (4.31)

using  $g_s$  from Eq. (2.9).

We may use the expression of Grotch and Hegstrom<sup>40</sup> to evaluate the hydrogen g factor:

$$g_{J}(H, 1^{2}S_{1/2}) = g_{S} \left\{ 1 - \frac{1}{3} \alpha^{2} \left[ 1 - \frac{3}{2} \frac{m}{M} + 3 \left( \frac{m}{M} \right)^{2} \right] + \frac{1}{4\pi} \alpha^{3} \left[ 1 - \frac{5}{3} \frac{m}{M} + \frac{7}{3} \left( \frac{m}{M} \right)^{2} \right] \right\},$$

$$(4.32)$$

where M is the proton mass. One obtains

$$g_J(H, 1^2S_{1/2}) = g_S(1 - 17.705 1 \times 10^{-6}).$$
 (4.33)

Hence from Eq. (4.31) and Eq. (4.33) the ratio is

$$\frac{g_{J}(\text{He}, 2^{3}\text{S}_{1})}{g_{J}(\text{H}, 1^{2}\text{S}_{1/2})} \bigg|_{\text{theory}} = 1 - 23.286 \, 92 \times 10^{-6}.$$
 (4.34)

(See "Note added in proof" at the end of the Appendix.)

A recent precise measurement by Brossel et al.<sup>17</sup> of the ratio of the magnetic moment in the  $2 {}^{3}S_{1}$  state of <sup>4</sup>He to the nuclear magnetic moment in the ground state of <sup>3</sup>He, when combined with other experimental measurements, yields a more precise ratio than that of Eq. (4.16),

$$\frac{g_{I}(\text{He}, 2^{3}\text{S}_{1})}{g_{J}(\text{H}, 1^{2}\text{S}_{1/2})} \bigg|_{\text{expt}} = 1 - (21.6 \pm 0.5) \times 10^{-6}. \quad (4.35)$$

The discrepancy between the theoretical value of Eq. (4.34) and experimental value of Eq. (4.35)is about three standard deviations of the experimental error. The Breit equation includes terms

TABLE V. Corrections to  $g_S$  factors in triplet states of helium.

$(g'_S - g_S)  imes 10^6$	
-81,983 22	
-80.462 23	
-75.121 51	
-73,29433	
-72.45957	

to order  $(Z\alpha)^2 \mu_B H$ . The next-higher-order term in the Zeeman effect has not been calculated for helium but should be of order  $\alpha^3 \mu_B H$ . The  $\alpha^3$  contribution to the g factor in the ground state of hydrogen,  $g_J(H, 1\,^2S_{1/2})$ , in Eq. (4.32) is  $\alpha^3/4\pi$ or about  $0.03 \times 10^{-6}$ . Thus an  $\alpha^3$  correction of this order of magnitude for helium would not eliminate the discrepancy between theory and experiment. Experiments to remeasure the g factor in 2 <sup>3</sup>S helium are in progress at Berkeley, at the Ecole Normale Superieure, and at Yale.

## D. Relativistic Contributions to the Magnetic Moment of Triplet States in Helium and Heliumlike Ions

We note that the expression for  $g'_s$  in Eq. (4.27) is valid for triplet states. The particular radial dependence of the wave function is, of course, important in the evaluation of the matrix elements. Table V presents the  $g'_s$  factors for five states of helium. We have used matrix elements calculated by Pekeris<sup>35,41,42</sup> for T and  $r_{12}^{-1}$ . It is very interesting to note that the use of Eq. (4.27) verifies our numerical wave-function calculation of  $g'_s$  in the 2<sup>3</sup>P state.

Table VI presents relativistic contributions, to order  $\alpha^2$ , to the *g* factors of heliumlike ions from Li II to Ne IX. Matrix elements calculated by Pekeris<sup>42</sup> were used in the application of Eq. (4.27).

## APPENDIX: EXPANSION OF POWERS OF THE INTERELECTRON DISTANCE

The expansion of powers of the interelectron distance  $r_{12}$  was discussed by Sack.<sup>33</sup> The series for  $r_{12}^{-1}$ ,

$$r_{12}^{-1} = r_{>}^{-1} \sum_{l=0}^{\infty} \left(\frac{r_{<}}{r_{>}}\right)^{l} P_{l}(\cos\theta_{12}), \tag{A1}$$

TABLE VI. Relativistic contributions, to order  $\alpha^2$ , to the g factors of heliumlike ions.  $(g'_S - g_S) \times 10^6$  is tabulated.

	2 <sup>3</sup> P <sub>1</sub>	3 <sup>3</sup> <b>P</b> <sub>1</sub>	4 <sup>3</sup> P <sub>1</sub>	5 <sup>3</sup> P <sub>1</sub>
Li <sup>7</sup> II	-187.52129	-171.9165	-166.548	-164.084
Be <sup>9</sup> III	-338.8803	-308.136	-297.51	-292.6
B <sup>11</sup> IV	-534.5915	-483.795	-466.19	-458.1
C <sup>12</sup> V	-774.6687	-698.897	-672.59	-660.47
N <sup>14</sup> VI	-1059.117	-953.44	-916.7	-899.77
O <sup>16</sup> VII	-1387.938	-1247.43	-1198.6	-1176.0
F <sup>19</sup> VIII	-1761.134	-1580.871	-1518.1	-1489.1
Ne <sup>20</sup> IX	-2178.705	-1953.752	-1875.39	-1839.2

is well known. Jen<sup>43</sup> gave the expansion for  $r_{12}$  in terms of Legendre polynomials:

$$r_{12} = r_{>} \sum_{l=0}^{\infty} \left[ \left( \frac{r_{<}}{r_{>}} \right)^{2} \frac{1}{2l+3} - \frac{1}{2l-1} \right] \left( \frac{r_{<}}{r_{>}} \right)^{l} P_{l}(\cos \theta_{12})$$
(A2)

Sack expanded  $r_{12}^n$  in terms of radial functions and Legendre polynomials:

$$r_{12}^{n} = \sum_{l=0}^{\infty} R_{nl}(r_{1}, r_{2}) P_{l}(\cos\theta_{12}).$$
 (A3)

The radial functions  $R_{nl}$  are defined in terms of the hypergeometric function:

$$F(\alpha,\beta;\gamma,x) = 1 + \sum_{1}^{\infty} \frac{(\alpha)_{s}(\beta)_{s}}{(\gamma)_{s}s!} x^{s}, \qquad (A4)$$

where

$$(\alpha)_0 = 1; \quad (\alpha)_s = \alpha(\alpha+1)\cdots(\alpha+s-1) = \Gamma(\alpha+s)/\Gamma(\alpha).$$

The  $R_{nl}$  are given by:

$$R_{nl}(r_1, r_2) = \frac{\left(-\frac{1}{2}n\right)_l}{\left(\frac{1}{2}\right)_l} r_{>}^n \left(\frac{r_{<}}{r_{>}}\right)^l \times F(l - \frac{1}{2}n, -\frac{1}{2} - \frac{1}{2}n; l + \frac{3}{2}, r_{<}^2/r_{>}^2).$$
(A5)

The hypergeometric functions (A4) are finite series if either  $\alpha$  or  $\beta$  is a negative integer or zero. Thus  $r_{12}^n$  can be expanded in a polynomial in  $(r_{\langle}/r_{\rangle})^l$  if *n* is a positive odd integer, and it can be shown that finite expansions are possible for negative odd integer *n*. Various recursion relations can be developed in the  $R_{nl}$ .

In addition to (A1) and (A2) we may explicitly write

$$r_{12}^{3} = 3r_{>}^{3}\sum_{l} \left(\frac{r_{<}}{r_{>}}\right)^{l} \left( [(2l-1)(2l-3)]^{-1} - 2[(2l-1)(2l+3)]^{-1} \left(\frac{r_{<}}{r_{>}}\right)^{2} + [(2l+3)(2l+5)]^{-1} \left(\frac{r_{<}}{r_{>}}\right)^{4} \right) P_{l}(\cos\theta_{12}), \quad (A6)$$

$$r_{12}^{5} = -15r_{>}^{5}\sum_{l} \left(\frac{r_{<}}{r_{>}}\right)^{l} \left( [(2l-5)(2l-3)(2l-1)]^{-1} - 3[(2l-3)(2l-1)(2l+3)]^{-1} \left(\frac{r_{<}}{r_{>}}\right)^{2} + 3[(2l-1)(2l+3)(2l+5)]^{-1} \left(\frac{r_{<}}{r_{>}}\right)^{4} - [(2l+3)(2l+5)(2l+7)]^{-1} \left(\frac{r_{<}}{r_{>}}\right)^{6} \right) P_{l}(\cos\theta_{12}), \quad (A7)$$

$$r_{12}^{7} = 105r_{5}^{7} \sum_{l} \left(\frac{r_{\varsigma}}{r_{5}}\right)^{l} \left( \left[ (2l-7)(2l-5)(2l-3)(2l-1)\right]^{-1} - 4\left[ (2l-5)(2l-3)(2l-1)(2l+3)\right]^{-1} \left(\frac{r_{\varsigma}}{r_{5}}\right)^{2} + 6\left[ (2l-3)(2l-1)(2l+3)(2l+5)\right]^{-1} \left(\frac{r_{\varsigma}}{r_{5}}\right)^{4} - 4\left[ (2l-1)(2l+3)(2l+5)(2l+7)\right]^{-1} \left(\frac{r_{\varsigma}}{r_{5}}\right)^{6} + \left[ (2l+3)(2l+5)(2l+7)(2l+9)\right]^{-1} \left(\frac{r_{\varsigma}}{r_{5}}\right)^{8} \right) P_{l}(\cos\theta_{12}),$$
(A8)

$$r_{12}^{-3} = \frac{1}{r_{2}^{2} - r_{1}^{2}} \sum_{l} \frac{r_{2}^{\prime}}{r_{2}^{l+1}} (2l+1) P_{l}(\cos\theta_{12}), \tag{A9}$$

$$r_{12}^{-5} = \frac{1}{3(r_{2}^{2} - r_{\zeta}^{2})^{3}} \sum_{l} \frac{r_{\zeta}^{l}}{r_{2}^{l+1}} \frac{(2l+1)[(2l+3)r_{2}^{2} - (2l-1)r_{\zeta}^{2}]P_{l}(\cos\theta_{12}).$$
(A10)

The expansion of  $r_{12}^{-2}$  contains series whose sums are logarithmic. The first two terms in the expansion are given by

$$r_{12}^{-2} = \frac{1}{2r_1r_2} \ln \frac{(r_1+r_2)}{|r_1-r_2|} + \left[ \frac{3}{4} \left( \frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \ln \frac{(r_1+r_2)}{|r_1-r_2|} - \frac{3}{2r_1r_2} \right] \cos \theta_{12} + \cdots$$
(A11)

These expansions are rather useful in the computation of radial and angular integrals.

Note added in proof. A new experimental determination of  $g_J(\text{He}, 2^3S_1)/g_J(\text{H}, 1^2S_{1/2})$  has recently been reported [E. Aygün, B. D. Zak, and H. A. Shugart, Phys. Rev. Lett. 31, 803 (1973)]:

$$\frac{g_J(\text{He}, 2^3S_1)}{g_J(\text{H}, 1^2S_{1/2})} = 1 - (23.25 \pm 0.30) \times 10^{-6}$$

8

This value is in excellent agreement with the theoretical value given in Eq. (4.34).

- \*Research supported in part by the Air Force Office of Scientific Research AFSC under AFOSR Contract No. F44620-70-C-0091.
- <sup>†</sup>Paper based in part on a dissertation submitted by M. L. Lewis in partial fulfillment of the requirements for the degree of Doctor of Philosophy at Yale University.
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