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 $2^{3}P$, $2^{3}S$, $3^{3}P$, 4³P, and 5³P states of helium is given. The contributions to the g factors g'_{S} , g'_{L} , and g_{X} , have been calculated to order α^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 2^3P 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 aine precisely the fine-structure constant α 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 α from the meation of the fine-structure constant α from the mesurement of the energy levels of the $2^{3}P$ state in a magnetic field.^{1,2} In this paper the contribution a magnetic field.^{1,2} In this paper the contribution 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 $4^{4}He$. $3-5$ 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 isoeleetronic series from Li II through Ne 1X are given.

The Hamiltonian for the Zeeman effect includes terms to order α^2 and m/M for helium and contains both relativistic and virtual radiative contributions to atomic magnetism. $8-8$ The way anomalous moments and relativistic contributions to the g factors combine in a composite system⁹ is of interest. Discrepancies are present between the theoretically and experimentally determined g factors for some many-electron atoms.¹⁰

The comparison of theoretical and experimental values^{1,2,11,12} of the fine-structure intervals and the Zeeman effect in the $2^{3}P$ state of helium is a significant test of the theory of two-electron atoms. It is of particular interest to test the twobody wave equation in states of nonzero orbital angular momentum since many terms in the Hamiltonian that vanish for S states are nonzero in P states.

The Zeeman Hamiltonian, accurate to order α^2 , was developed from a modified Breit equa- μ , was developed from a modified Breft equation 13 by Perl and Hughes, 6 Abragam and Van Vleck, 14 and Kambe and Van Vleck.¹⁵ Many s Vleck,¹⁴ and Kambe and Van Vleck.¹⁵ Many similar operators appear in the fine-structure Hamiltonian and hence the fine-structure interval may be calculated by methods used here.¹⁶

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. '6 The extrapolated value of the energy from the calculation of the wave function is accurate to better than one part in 10'. 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 $2³S_J$ helium by Brossel et $al.^{17}$ and the previous calhelium by Brossel *et al*.¹⁷ and the previous cal-
culation⁶ and experiment.¹⁸ In an attempt to verify and improve the calculation by Perl and Hughes $⁶$ </sup> of the g_J factor in the $2³S₁$ 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

8

hypergeometric functions and Legendre polynomials. Brief reports of this research have been presented.^{3,5} etr
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3.5

II. ZEEMAN HAMILTONIAN

The Zeeman Hamiltonian for helium can be The Zeeman Hamiltonian for helium can be
developed from the Breit equation.¹⁹ The theoretical development of the reduced Hamiltonian was due to Perl and Hughes,⁶ Abragam and Van was due to Perl and Hughes,⁶ Abragam and Var
Vleck,¹⁴ and Kambe and Van Vleck.¹⁵ Innes and Ufford'0 re-expressed the Zeeman Hamiltonian Ufford²⁰ re-expressed the Zeeman Hamiltonian
in spherical-tensor notation.²¹ The use of spheri cal tensors greatly facilitates the calculation of the g factors.²⁰

A. The Breit Equation

In order to apply the theory to more general cases than two-electron atoms, we write the Breit equation¹³ as

$$
\mathcal{K}_B = \sum_i (\vec{\alpha}_i \cdot \vec{p}_i + \beta_i m - Ze^2/\gamma_i)
$$
\n
$$
+e^2 \sum_{i \le j} \left(\frac{1}{\gamma_{ij}} - \frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{2\gamma_{ij}} - \frac{\vec{\alpha}_i \cdot \vec{r}_{ij} \cdot \vec{\alpha}_j \cdot \vec{r}_{ij}}{2\gamma_{ij}^3} \right),
$$
\n
$$
+e^2 \sum_{i \le j} \left(\frac{1}{\gamma_{ij}} - \frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{2\gamma_{ij}} - \frac{\vec{\alpha}_i \cdot \vec{r}_{ij} \cdot \vec{\alpha}_j \cdot \vec{r}_{ij}}{2\gamma_{ij}^3} \right),
$$
\nThis is equivalent to the use of a
\ntonian²⁵ that includes radiative eff

where for helium the sum is over two electrons. In \mathcal{K}_n , \bar{r}_i is the position of the *i*th electron, \bar{p}_i is the momentum, α_i and β_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, \vec{p}_i is replaced by $\vec{p}_i + e \vec{A}(\vec{r}_i)$.

The Breit Hamiltonian is reduced to large components by standard techniques^{13,22} to order $(Z\alpha)^2$ Hy. The magnetic-field-dependent terms have Ry. The magnetic-field-dependent terms have
been retained to order $(Z\alpha)^2\mu_B H$ by Perl⁷ and
Abragam and Van Vleck.¹⁴ The latter paper i Abragam and Van Vleck.¹⁴ 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{X}_z contains seven terms:

$$
\mathcal{K}_z = \sum_{i=0}^{6} \mathcal{K}_i , \qquad (2.2)
$$

$$
\mathcal{K}'_0 = \mu_B \vec{H} \cdot (\vec{L} + g_S \vec{S}), \tag{2.3}
$$

$$
\mathcal{K}_1 = -\alpha^2 \mu_B \vec{H} \cdot \sum_i (\vec{I}_i + 2\vec{S}_i) T_i , \qquad (2.4)
$$

$$
\mathcal{K}_2 = \frac{1}{2} Z \alpha^2 \mu_B \vec{H} \cdot \sum_i \left[\vec{s}_i \times \vec{\nabla}_i (\ r_i^{-1}) \right] \times \vec{r}_i, \tag{2.5}
$$

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

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

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

The vector potential $\vec{A}(\vec{r})$ has been set equal to $\frac{1}{2}H \times \vec{r}_i$. \mathcal{K}_0 is the lowest-order Zeeman effect. Here $\tilde{\mathbf{L}}$ = $\sum_i \vec{\mathbf{l}}_i$ is the total orbital angular momen tum and $\bar{\mathbf{S}} = \sum_i \bar{\mathbf{s}}_i$ is the total spin. \mathcal{K}_1 is analogou to the relativistic increase of mass and T_i is the kinetic energy of the ith electron. The reduction of the Breit equation (2.1) yields \mathcal{X}_2 , \mathcal{X}_3 , \mathcal{X}_4 , and $3C₅$, which include terms analogous to spin-orbit \mathcal{X}_5 , which include terms analogous to spin-orbit,
spin-other-orbit, and orbit-orbit interactions.^{14,15} The last term in the Zeeman Hamiltonian \mathcal{K}'_6 includes a correction for the motion of the center
of mass,²³ where M is the atomic mass. of mass,²³ where M is the atomic mass

Radiative corrections are included by using the gyromagnetic ratio of the free electron²⁴ g_s :

$$
\frac{1}{2}(g_S - 2) = \alpha/2\pi - 0.32848(\alpha/\pi)^2
$$

+ (1.29 \pm 0.06)(\alpha/\pi)^3. (2.9)

This is equivalent to the use of a Pauli Hamiltonian²⁵ that includes radiative effects.

B. Spherical- Tensor Notation

Innes and Ufford²⁰ recoupled the operators \mathcal{R}_i
to spherical-tensor notation.²¹ We define a into spherical-tensor notation. We define a tensor $C_a^{(k)}$ 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 \mathcal{K}'_6 : $-(m/M)\mu_B\vec{H}\cdot\vec{L}$, define $g_L = 1 - m/M$, and rewrite \mathcal{K}_0 as

$$
\mathcal{K}_o = \mu_B \vec{H} \cdot (g_L \vec{L} + g_S \vec{S}). \tag{2.11}
$$

With the notation

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

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

$$
\mathcal{K}_o = \mu_B \vec{H} \cdot (g_L \vec{L} + g_S \vec{S}), \tag{2.12}
$$

$$
\mathcal{K}_1 = -\alpha^2 \mu_B \vec{\mathbf{H}} \cdot \sum_i (\vec{\mathbf{I}}_i + 2\vec{\mathbf{s}}_i) T_i , \qquad (2.13)
$$

$$
\mathcal{K}_2 = \frac{2}{3} \alpha^2 \mu_B \vec{H} \cdot \sum_i \frac{1}{r_i} \left[\vec{s}_i + (\frac{5}{2})^{1/2} \{\vec{s}_i C_i^{(2)}\}^{(1)} \right], (2.14)
$$

$$
3C_3 + 3C_4 = 2\alpha^2 \mu_B \vec{H} \cdot \sum_{i \le j} \left\{ (\vec{s}_i + 2\vec{s}_j) \sum_k (-1)^k (2k+1)^{1/2} \times \left[\frac{1}{3} \left(k \frac{\epsilon_{ij} r_1^k}{r_j^{k+1}} - (k+1) \frac{\epsilon_{ji} r_1^k}{r_i^{k+1}} \right) \left\{ C_i^{(k)} C_j^{(k)} \right\}^{(0)} + \frac{\left[k(k+1) \right]^{1/2}}{2\sqrt{6}} \left(\frac{\epsilon_{ij} r_1^k}{r_j^{k+1}} + \frac{\epsilon_{ji} r_1^k}{r_i^{k+1}} \right) \left\{ C_i^{(k)} C_j^{(k)} \right\}^{(1)} - \frac{\left[k(k+1) \right]^{1/2}}{6\sqrt{2}} \left(\left(\frac{2k+3}{2k-1} \right)^{1/2} \frac{\epsilon_{ij} r_1^k}{r_j^{k+1}} - \left(\frac{2k-1}{2k+3} \right)^{1/2} \frac{\epsilon_{ji} r_1^k}{r_i^{k+1}} \right) \left\{ C_i^{(k)} C_j^{(k)} \right\}^{(2)} + \frac{1}{2\sqrt{3}} \left(\frac{k(k-1)(2k-3)}{2k-1} \right)^{1/2} \frac{\epsilon_{ij} r_1^k}{r_j^{k+1}} \left\{ C_i^{(k-2)} C_j^{(k)} \right\}^{(2)} - \frac{1}{2\sqrt{3}} \left(\frac{(k+1)(k+2)(2k+5)}{2k+3} \right)^{1/2} \frac{\epsilon_{ij} r_1^k}{r_i^{k+1}} \left\{ C_i^{(k+2)} C_j^{(k)} \right\}^{(2)} \right\}^{\binom{11}{2}}, \qquad (2.15)
$$

$$
\mathcal{K}_{5} = \frac{1}{\sqrt{3}} \alpha^{2} \mu_{B} \vec{H} \cdot \sum_{i \leq j} \sum_{k} (-1)^{k} \left\{ \left(\frac{\epsilon_{ji} r_{j}^{k}}{r_{i}^{k+1}} + \frac{\epsilon_{ij} r_{i}^{k+2}}{r_{j}^{k+3}} \right) \right. \\ \times \left\{ \frac{k(k+3)}{2k+3} \left[(2k+1)^{1/2} \left\{ C_{i}^{(k)} \left[C_{j}^{(k)} \vec{1}_{j} \right\}^{(k)} \right\}^{(1)} - (2k+5)^{1/2} \left\{ C_{i}^{(k+2)} \left[C_{j}^{(k+2)} \vec{1}_{j} \right\}^{(k+2)} \right\}^{(1)} \right] \right. \\ \left. - 2 \left(\frac{2k+1}{2k+3} \right)^{1/2} \left[(2k+1)^{1/2} \left\{ C_{i}^{(k)} \left[C_{j}^{(k)} \vec{1}_{j} \right\}^{(k+1)} \right\}^{(1)} + \left(\frac{(k+1)(2k+5)}{k+2} \right)^{1/2} \left\{ C_{i}^{(k+2)} \left[C_{j}^{(k)} \vec{1}_{j} \right\}^{(k+1)} \right\}^{(1)} \right] \right) \right. \\ \left. + \left((k+3) \frac{\epsilon_{ij} r_{j}^{k+2} \partial r_{j}}{r_{j}^{k+2}} - k \frac{\epsilon_{ji} r_{j}^{k+1} \partial r_{j}}{r_{i}^{k+1}} \right) \frac{1}{2k+3} \right. \\ \times \left\{ \left[k(k+1)(2k+1) \right]^{1/2} \left\{ C_{i}^{(k)} C_{j}^{(k)} \right\}^{(1)} - \left[(k+2)(k+3)(2k+5) \right]^{1/2} \left\{ C_{i}^{(k+2)} C_{j}^{(k+2)} \right\}^{(1)} \right\} \right\} ,
$$

$$
(2.16)
$$

$$
\mathcal{K}_{6} = -2(m/M)\mu_{B}\vec{H} \cdot \sum_{i \leq j} \left[2(r_{i}/r_{j})\left\{C_{i}^{(1)}\left\{C_{j}^{(1)}\right\}\right\}^{(1)}\right\}^{(1)} - \sqrt{2} r_{i} \partial r_{j} \left\{C_{i}^{(1)}C_{j}^{(1)}\right\}^{(1)}\right].
$$
\n(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 26.27 have been used to approximate the helium eigenvalues and eigenfunctions. Bartlett²⁸ and eigenvalues and eigenfunctions. Bartiett⁻⁻ and
Gronwall²⁹ demonstrated that these expansions do not solve the Schrddinger 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 30 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 $2^{3}P$ Helium

The wave function Ψ_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 as¹⁶

$$
U_{lmn}(1,2) = \frac{1-P_{12}}{4\pi\sqrt{2}} \tilde{r}_1 r_1^m r_2^n r_{12}^l
$$

× $e^{-\kappa \sigma/2} r_1 e^{-(\kappa/2)r_2}$. (3.2)

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

$$
\Psi_0 = \sum_{i, m, n=0}^{i + m + n \leq \omega} C_{i m n} U_{i m n} (1, 2),
$$
\n(3.3)

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

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

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

The interelectron distance is

$$
r_{12} = |\vec{r}_1 - \vec{r}_2|
$$

= $(r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12})^{1/2}$, (3.5)

where θ_{12} is the angle between \mathbf{r}_1 and \mathbf{r}_2 .

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

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

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

TABLE I. Ordering of terms in Hylleraas basis.

\boldsymbol{N}	ı	\boldsymbol{m}	n	$\boldsymbol{\omega}$
$\mathbf{1}$	0	0	$\bf{0}$	0
$\overline{\mathbf{c}}$	$\bf{0}$	0	1	1
3	0	$\mathbf{1}$	0	1
$\overline{4}$	$\mathbf{1}$	0	$\bf{0}$	$\mathbf{1}$
5	$\bf{0}$	$\bf{0}$	2	$\bf{2}$
6	$\bf{0}$	$\mathbf{1}$	$\mathbf{1}$	$\overline{\mathbf{2}}$
7	$\bf{0}$	$\overline{\mathbf{2}}$	$\bf{0}$	$\overline{\mathbf{2}}$
8	$\mathbf{1}$	$\bf{0}$	$\mathbf{1}$	$\overline{\mathbf{2}}$
9	$\mathbf{1}$	1	$\bf{0}$	$\overline{2}$
10	$\overline{\mathbf{2}}$	$\bf{0}$	$\pmb{0}$	$\mathbf 2$
11	$\bf{0}$	$\bf{0}$	3	3
12	$\bf{0}$	$\mathbf{1}$	$\overline{\mathbf{2}}$	3
13	$\bf{0}$	$\overline{\mathbf{c}}$	$\mathbf{1}$	3
14	0	3	$\bf{0}$	3
15	$\mathbf{1}$	0	$\boldsymbol{2}$	3
16	1	$\mathbf{1}$	1	3
17	$\mathbf{1}$	$\overline{2}$	$\mathbf 0$	3
18	$\overline{\mathbf{2}}$	$\bf{0}$	1	3
19	$\boldsymbol{2}$	$\mathbf{1}$	0	3
20	3	$\bf{0}$	0	3
21	$\bf{0}$	0	4	$\overline{\mathbf{4}}$
22	$\bf{0}$	1	3	$\overline{\mathbf{4}}$
23	$\bf{0}$	$\overline{\mathbf{2}}$	$\mathbf 2$	$\overline{\mathbf{4}}$
24	$\bf{0}$	3	$\mathbf{1}$	$\overline{\bf 4}$
25	$\bf{0}$	$\overline{\bf 4}$	0	$\overline{\mathbf{4}}$
26	$\mathbf{1}$	0	3	$\overline{\mathbf{4}}$
27	$\mathbf{1}$	1	$\overline{\mathbf{2}}$	$\overline{\mathbf{4}}$
28	1	$\overline{\mathbf{2}}$	$\mathbf 1$	$\overline{\mathbf{4}}$
29	$\mathbf{1}$	3	$\bf{0}$	$\overline{\textbf{4}}$
30	2	$\bf{0}$	$\mathbf 2$	$\overline{\mathbf{4}}$
31	$\overline{\mathbf{2}}$	$\mathbf{1}$	$\frac{1}{0}$	$\overline{\mathbf{4}}$
32	$\overline{\mathbf{2}}$	$\overline{\mathbf{2}}$		$\overline{\mathbf{4}}$
33	3	$\bf{0}$	$\mathbf{1}$	$\overline{\mathbf{4}}$
34	3	1	0	$\overline{\mathbf{4}}$
35	$\overline{\mathbf{4}}$	$\bf{0}$	$\bf{0}$	$\overline{\mathbf{4}}$

lowest-order approximation.

We have calculated wave functions for the index ω in Eq. (3.3) from one through eight. The total number of terms in a wave function for a given ω 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 $\omega \le 4$.

We have used the screening parameters κ and σ given by Schwartz¹⁶:

$$
\kappa = 4.619\,999\,945\,163\,72,\tag{3.7}
$$

$$
\sigma = 0.2899999999105930. \tag{3.8}
$$

These values may be compared to the results in an early calculation by Eckart³¹ and reported in a different form:

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

$$
\sigma_E = 0.27. \tag{3.10}
$$

The energy eigenvalue of $2³P$ helium obtained from our variational calculation is presented in Table II. The extrapolated energy is in excellent agreement with Schwartz's best result¹⁶ of -2.133164 1908 a.u. These wave functions were calculated in double. precision on an IBM 360/67 machine.

B. Integrals

Many integrals" are needed to calculate the matrix elements of \mathcal{X}_i with Ψ_0 in Eq. (3.3). The major ones are

$$
A(L, M, N) = \int \frac{d\tau_1}{4\pi} \int \frac{d\tau_2}{4\pi} e^{-\mathbf{a}\mathbf{r}_1} e^{-\mathbf{b}\mathbf{r}_2}
$$

× $r_1^{M-2} r_2^{N-2} r_{12}^{L-2}$, (3.11)

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

N	Energy $(a.u.)$
1	-2.072137762
2	-2.123103128
4	-2.129471788
10	-2.132678402
20	-2.133085039
35	-2.133140222
56	-2.133157595
84	-2.133162287
120	-2.133163594
165	-2.133163981
Extrapolated	-2.1331642

$$
B(L, M, N) = \int \frac{d\tau_1}{4\pi} \int \frac{d\tau_2}{4\pi} e^{-a\tau_1} e^{-b\tau_2}
$$

$$
\times r_1^{\mu-2} r_2^{\mu-2} r_{12}^{L-2} \cos \theta_{12} . \tag{3.12}
$$

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

 $\pmb{8}$

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

These relations may be obtained with

 \mathbb{R}^n and \mathbb{R}^n

$$
r_{12}^2 = r_1^2 + r_2^2 - 2r_1r_2\cos\theta_{12} \tag{3.15}
$$

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

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

then we may show

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

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

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

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

The F integrals are calculated using

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

$$
F(M, N; \alpha, \beta) = \frac{(M + N - 2)!}{\beta (\alpha + \beta)^{M + N - 1}} + \frac{N - 1}{\beta} F(M, N - 1; \alpha, \beta).
$$
\n(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 $Sack³³$ is discussed.

The lowest-order term in the expansion

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

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

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

$$
A_e(0, M, N) = \frac{1}{2} \left[F_{1c}(M, N) + F_{1c}(N, M) \right]; \tag{3.26}
$$

$$
B_{d}(0, M, N) = \frac{1}{4} \left[F_{la}(M+1, N-1) + F_{la}(M-1, N+1) + F_{Io}(N+1, M-1) + F_{Ib}(N-1, M+1) \right]
$$

+
$$
F_{lo}(N+1, M-1) + F_{Ib}(N-1, M+1) \right]
$$

-
$$
\frac{1}{2} \left[F(M, N; \kappa \sigma, \kappa) + F(N, M, \kappa, \kappa \sigma) \right],
$$

(3.27)

$$
B_e(0, M, N) = \frac{1}{4} \left[F_{tc}(M+1, N-1) + F_{tc}(M-1, N+1) + F_{tc}(N+1, M-1) + F_{tc}(N-1, M+1) \right]
$$

$$
- \frac{1}{2} \left[F(M, N; \delta, \delta) + F(N, M; \delta, \delta) \right],
$$

(3.28)

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

$$
F_t(M, N; \alpha, \beta) = \int_0^{\infty} dr \, e^{-\alpha r} \, r^{M-1}
$$

$$
\times \int_r^{\infty} ds \, e^{-\beta s} \, s^{M-1} \ln \frac{s+r}{s-r} \,, \quad (3.29)
$$

and

$$
F_{1a}(M, N) = F_{1}(M, N; \kappa\sigma, \kappa),
$$

\n
$$
F_{1b}(M, N) = F_{1}(M, N; \kappa, \kappa\sigma),
$$

\n
$$
F_{1c}(M, N) = F_{1}(M, N; \delta, \delta).
$$
\n(3.30)

The F_t integrals may be written as sums of prod-
ucts of various functions.³² ucts of various functions.

For the A and B integrals with $M=0$, $N\geq 1$ 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 2^3S_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^{16,34} is

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

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

$$
v_{LMN}(1, 2) = (1 - \frac{1}{2}Z_b \gamma_2) e^{-(Z_a/2)\gamma_1}
$$

$$
\times e^{-(Z_b/2)\gamma_2} \gamma_1^M \gamma_2^N \gamma_{12}^L.
$$

For a preliminary 35-term wave function we obtained $E = -2.175212$ a.u., which is in adequate agreement with the result of Pekeris³⁵ 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,³⁶ who obtained the results of Traub and Foley,³⁶ who obtaine $Z_a = 4.12$ and $Z_b = 1.20$.

IV. RESULTS AND DISCUSSION

A. Hydrogenic Approximation for 2^3P Helium

We approximate the helium wave function with a product of 1s and $2p$ hydrogenic wave function
and calculate the Zeeman effect.¹² and calculate the Zeeman effect.

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 χ includes spin variables, $\boldsymbol{\Omega}$ includes the angular variables,

$$
R_{1s}(r_i) = R_{10}(r_i)
$$

= $2Z_1^{3/2}e^{-Z_1r_i}$

and

$$
R_{2p}(r_i) = R_{21}(r_i)
$$

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

The values of the screening constants are The values of the screening constants are
 $Z_1 = 1.99$, $Z_2 = 1.09$.³¹ Z_1 and Z_2 are related to κ and σ in Eq. (3.2):

$$
\kappa = 2Z_1 = 3.98, \n\sigma = Z_2/2Z_1 = 0.27.
$$
\n(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 $\langle \, ^3P_J m_J | \, ^3C_Z | \, ^3P_J m_J \rangle$ is given in terms of radia
integrals R_i and various n -j symbols:

$$
\langle |\mathcal{K}_0| \rangle = \sqrt{6} \ \mu_B H (-1)^{1 - m_J} (2J + 1)^{1/2} (2J' + 1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_J & 0 & m_J \end{pmatrix} \begin{cases} J & 1 & J' \\ 1 & 1 & 1 \end{cases} [(-1)^{J + J'} g_L + g_S], \tag{4.4}
$$

$$
\langle |\mathcal{K}_1| \rangle = -\sqrt{6} \ \alpha^2 \mu_B H (-1)^{1 - m} J (2J + 1)^{1/2} (2J' + 1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_J & 0 & m_J \end{pmatrix} \begin{cases} J & 1 & J' \\ 1 & 1 & 1 \end{cases} \{R_1 + [1 + (-1)^{J + J'}] R_2\},
$$
(4.5)

$$
\langle |\mathcal{K}_2| \rangle = \sqrt{6} \alpha^2 \mu_B H (-1)^{1 - m} J (2 J + 1)^{1/2} (2 J' + 1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_J & 0 & m_J \end{pmatrix}
$$

$$
\times \left(\frac{1}{3} \begin{pmatrix} J & 1 & J' \\ 1 & 1 & 1 \end{pmatrix} (R_3 + R_4) + (-1)^J \begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 1 \\ J & J' & 1 \end{pmatrix} R_4 \right),
$$
 (4.6)

$$
\langle |\mathcal{K}_3 + \mathcal{K}_4| \rangle = \sqrt{6} \alpha^2 \mu_B H (-1)^{J - m} J (2J + 1)^{1/2} (2J' + 1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_J & 0 & m_J \end{pmatrix}
$$

$$
\times \left(\begin{array}{ccc} \begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 1 \\ J & J' & 1 \end{pmatrix} & \left(\frac{3}{2} R_6 + 2R_7 - \frac{3}{2} R_8 \right) + \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ J & J' & 1 \end{pmatrix} & (R_7 - \frac{3}{2} R_6 - \frac{3}{2} R_5) \right), \tag{4.7}
$$

$$
\langle |\mathcal{K}_5| \rangle = \sqrt{6} \alpha^2 \mu_B H (-1)^{J + J' + 1 - m_J} (2 J + 1)^{1/2} (2 J' + 1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_J & 0 & m_J \end{pmatrix}
$$

$$
\times \begin{pmatrix} J & 1 & J' \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} -\frac{1}{3} R_5 + \frac{2}{15} R_7 - \frac{1}{3} R_8 + \frac{2}{15} R_9 + \frac{1}{30} R_{10} - \frac{1}{30} R_{11} - \frac{2}{15} R_{12} + \frac{2}{15} R_{13} \end{pmatrix},
$$
 (4.8)

 (4.2)

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

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

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

 $\ddot{}$

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

$$
R_{1} = \langle |T_{1}| \rangle_{D_{sp}} = 1.98, \quad R_{2} = \langle |T_{1}| \rangle_{D_{sp}} = 0.149, \quad R_{3} = \langle \left| \frac{1}{r_{1}} \right| \rangle_{D_{sp}} = 1.99,
$$
\n
$$
R_{4} = \langle \left| \frac{1}{r_{1}} \right| \rangle_{D_{ps}} = 0.273, \quad R_{5} = \langle \left| \frac{1}{r_{1}} \right| \rangle_{D_{sp}} \quad (r_{2} \leq r_{1}) = 0.0046,
$$
\n
$$
R_{6} = \langle \left| \frac{1}{r_{1}} \right| \rangle_{D_{ps}} \quad (r_{2} \leq r_{1}) = 0.267, \quad R_{7} = \langle \left| \frac{r_{1}}{r_{2}^{2}} \right| \rangle_{E} \quad (r_{1} \leq r_{2}) = 0.0079,
$$
\n
$$
R_{8} = \langle \left| \frac{r_{1}^{2}}{r_{2}^{3}} \right| \rangle_{D_{sp}} \quad (r_{1} \leq r_{2}) = 0.025, \quad R_{9} = \langle \left| \frac{r_{1}^{3}}{r_{2}^{4}} \right| \rangle_{E} \quad (r_{1} \leq r_{2}) = 0.0043,
$$
\n
$$
R_{10} = \langle \left| \frac{r_{2}^{2} \partial r_{2}}{r_{1}^{2}} \right| \rangle_{E_{ps}} \quad (r_{2} \leq r_{1}) = 0.003, \quad R_{11} = \langle \left| \frac{r_{2}^{2} \partial r_{2}}{r_{1}^{2}} \right| \rangle_{E_{sp}} \quad (r_{2} \leq r_{1}) = -0.0177,
$$
\n
$$
R_{12} = \langle \left| \frac{r_{1}^{3} \partial r_{2}}{r_{2}^{3}} \right| \rangle_{E_{ps}} \quad (r_{1} \leq r_{2}) = 0.0007, \quad R_{13} = \langle \left| \frac{r_{1}^{3} \partial r_{2}}{r_{2}^{3}} \right| \rangle_{E_{sp}} \quad (r_{1} \leq r_{2}) = -0.0133,
$$
\n
$$
R_{14} = \langle |r_{1}^{2}|
$$

These radial integrals differ slightly from the previous calculation. $^{12,\,37}$

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

$$
\langle Jm_J \, | \mathcal{K}_Z | \, J'm_J \rangle = (-1)^{1-m_J} (2J+1)^{1/2} (2J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_J & 0 & m_J \end{pmatrix} \sqrt{6}
$$

$$
\times \left[\begin{array}{ccc} \{J & 1 & J' \\ 1 & 1 & 1 \end{array} \left\{ g'_s + (-1)^{J'+J'} g'_L \right\} + \begin{array}{ccc} 1 & 1 & 2 \\ 1 & 1 & 1 \\ J & J' & 1 \end{array} \left\{ (-1)^J g_x \right\} \mu_B H, \tag{4.10}
$$

where

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

+ $(m/M)(\frac{1}{3}R_{16} - \frac{1}{3}R_{17} + \frac{2}{3}R_{18});$

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

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

The g factor g_x , of order α^2 , comes from the matrix elements of a tensor composed of a spin vector and a spherical tensor of rank 2 such as $\{ \mathbf{\bar{S}} C^{(2)} \}^{(1)}$, 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

$$
g'_{s} = g_{s} - 80.3 \times 10^{-6},
$$

\n
$$
g'_{L} = g_{L} + 3.8 \times 10^{-6},
$$

\n
$$
g_{x} = -5.6 \times 10^{-6}.
$$
\n(4.12)

This result may be compared to the hydrogenic approximation¹² using less precise radial integrals

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

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

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

 $\pmb{8}$

B. Matrix Elements Using the Numerical Wave Function for $2³P$ 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{K}_0 has no radial or angular parts; hence we obtain the same result as Eq. (4.4):

$$
({}^{3}P_{J}m_{J} | \mathcal{K}_{0} | {}^{3}P_{J} \cdot m_{J})
$$

= $\sqrt{6} \mu_{B} H(-1)^{1-\pi_{J}} (2J+1)^{1/2} (2J'+1)^{1/2} {\begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix}}$
 $\times {\begin{pmatrix} J & 1 & J' \\ 1 & 1 & 1 \end{pmatrix}} [g_{S} + (-1)^{J+J'} g_{L}].$ (4.13)

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

$$
({}^{3}P_{J}m_{J} | \mathcal{K}_{Z} | {}^{3}P_{J}, m_{J})
$$

= $\sqrt{6} (-1)^{1-m_{J}} (2J+1)^{1/2} (2J'+1)^{1/2} \begin{pmatrix} J & 1 & J' \\ -m_{J} & 0 & m_{J} \end{pmatrix}$

$$
\times \begin{bmatrix} \begin{bmatrix} J & 1 & J' \\ 1 & 1 & 1 \end{bmatrix} [g'_{S} + (-1)^{J+J'} g'_{L}] \end{bmatrix}
$$

+ $\begin{bmatrix} 1 & 1 & 2 \\ 1 & 1 & 1 \\ J & J' & 1 \end{bmatrix} (-1)^{J} g_{X} \end{bmatrix} \mu_{B} H.$ (4.14)

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) configuracited comigurations as well as the (sp) comiguration—but this does not change the Zeeman Hamil-
tonian matrix.¹² tonian matrix.

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. 32 Essentially

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

Terms	$(g'_S - g_S) \times 10^6$	$(g_L' - g_L) \times 10^6$	$g_{\text{X}} \times 10^6$
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 ± 0.01	10.6 ± 0.4	-3.5 ± 2.5

the g factors are considered a function of the index ω , 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 ω is increased.

We can compare the result of this calculation with the hydrogenic approximations given in Eq. with the hydrogenic approximations given in Eq. (4.12) and the experimentally determined values.¹² 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_r 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 $2^{3}P_{I}$ helium would be useful. The measurement of the g factors in $2³P$ helium¹² is important for the determination of the 2^3P_1 - 2^3P_2 and 2^3P_1 - 2^3P_0 fine-structure inof the $2^{3}P_1$ ¹²

The $2^{1}P_{1}$ state of helium lies 6×10^{4} GHz above the $2^{3}P_{J}$ states. Spin-orbit interaction between states of the same total angular momentum J leads to a partial breakdown of $L-S$ coupling. Araki³⁸ and Pekeris³⁹ have shown that the singlet admixture shifts the energy of the $2^{3}P$, state by about 4.5 MHz. Second-order perturbationa from the singlet state do not contribute because the Hamiltonian \mathcal{R}_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.

	$(g'_S - g_S) \times 10^6$
Extrapolated	-80.46 ± 0.01
Hydrogenic	-80.3
Experiment	-76.0 ± 2.4
	$(g_L' - g_L) \times 10^6$
Extrapolated	10.6 ± 0.4
Hydrogenic	3.8
Experiment	3.8 ± 9.0
	$g_X \times 10^6$
Extrapolated	-3.5 ± 2.5
Hydrogenic	-5.6
Experiment	4.0 ± 25.0

$$
\frac{\langle {}^{3}P_{1}|spin-orbit| {}^{1}P_{1}\rangle\langle {}^{1}P_{1}|{}^{3}C_{Z}|{}^{1}P_{1}\rangle\langle {}^{1}P_{1}|spin-orbit|{}^{3}P_{1}\rangle}{[E(2 {}^{3}P_{1})-E(2 {}^{1}P_{1})]^{2}}.
$$
\n(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 $2³S₁$ Helium

Perl and Hughes⁶ evaluated the relativistic contributions to the magnetic moment of $2 \, \mathrm{^{3}S_{1}}$ helium. tributions to the magnetic moment of $2^{3}S_{1}$ heli
Drake *et al*.¹⁸ 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

$$
\frac{g_I(\text{He}, 2^3S_1)}{g_J(\text{H}, 1^2S_{1/2})}\bigg|_{\text{expt}} = 1 - (23.3 \pm 0.8) \times 10^{-6}. \quad (4.16)
$$

The theoretical ratio is⁶

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

The Zeeman Hamiltonian in Eqs. (2.12)-(2.17) can be used to find the g factor of the $2³S₁$ state of helium.

Matrix elements of the Zeeman Hamiltonian yield

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

$$
(\mathcal{E}_1|\mathcal{E}_1|\mathcal{E}_1) = -\alpha^2 \mu_B H(T), \qquad (4.19)
$$

$$
({}^3S_1|\mathcal{K}_2|{}^3S_1) = \frac{1}{3}\alpha^2\mu_B H\left(\left\langle\frac{1}{r_1}\right\rangle + \left\langle\frac{1}{r_2}\right\rangle\right),\tag{4.20}
$$

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

$$
({}^{3}S_{1}|{}^{3}C_{5}|{}^{3}S_{1})=0, \qquad (4.22)
$$

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

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

$$
({}^{3}S_{1}|\mathcal{K}_{Z}|{}^{3}S_{1}) = \mu_{B}H\left[g_{S} + \alpha^{2}\left(\frac{1}{3}\left\langle\frac{1}{r_{1}}\right\rangle\right) + \frac{1}{3}\left\langle\frac{1}{r_{2}}\right\rangle - \langle T \rangle - \frac{1}{2}\left\langle\frac{1}{r_{12}}\right\rangle\right)\right].
$$
\n(4.24)

⁴)
-By the use of the virial theorem,¹⁹ one can es tablish

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

Hence

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

where

$$
g'_s = g_s - 2\alpha^2 \left(\frac{1}{3} \langle T \rangle + \frac{1}{6} \left\langle \frac{1}{r_{12}} \right\rangle \right). \tag{4.27}
$$

This result agrees exactly with the calculation of Perl and Hughes.⁶ Pekeris³⁵ has calculated the value of the matrix elements of T and r_{12}^{-1} using a wave function with 715 terms:

$$
\langle T \rangle = 2.175\,229\,378\,24,\tag{4.28}
$$

$$
\left\langle \frac{1}{r_{12}} \right\rangle = 0.2681978553. \tag{4.29}
$$

Hence, using Eq. (4.27), the value for g'_{s} is

$$
g'_s = g_s - 81.98322 \times 10^{-6}.
$$
 (4.30)

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

$$
g_J
$$
(He, 2³S₁) = g_S (1 – 40.99161×10⁻⁶), (4.31)

using g_s from Eq. (2.9).

We may use the expression of Grotch and Hegstrom⁴⁰ to evaluate the hydrogen g factor:

$$
g_J(H, 1^2S_{1/2}) = g_S \left\{ 1 - \frac{1}{3} \alpha^2 \left[1 - \frac{3}{2} \frac{m}{M} + 3 \left(\frac{m}{M} \right)^2 \right] + \frac{1}{4\pi} \alpha^3 \left[1 - \frac{5}{3} \frac{m}{M} + \frac{7}{3} \left(\frac{m}{M} \right)^2 \right] \right\},
$$
\n(4.32)

where M is the proton mass. One obtains

$$
g_J(H, 1^2S_{1/2}) = g_S(1 - 17.7051 \times 10^{-6}). \qquad (4.33)
$$

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

$$
\frac{g_I(\text{He}, 2^3S_1)}{g_J(\text{H}, 1^2S_{1/2})}\bigg|_{\text{theory}} = 1 - 23.28692 \times 10^{-6}. \quad (4.34)
$$

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

A recent precise measurement by Brossel A recent precise measurement by Brossel
 *et al.*¹⁷ of the ratio of the magnetic moment in the $2³S₁$ state of ⁴He to the nuclear magnetic moment in the ground state, of 3 He, when combined with other experimental measurements, yields a more precise ratio than that of Eq. (4.16) ,

$$
\frac{g_I(\text{He}, 2^{3}S_1)}{g_J(\text{H}, 1^{2}S_{1/2})}\Big|_{\text{expt}} = 1 - (21.6 \pm 0.5) \times 10^{-6}. \quad (4.35)
$$

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.

	$(g'_S - g_S) \times 10^6$	
$2^{3}S_{1}$	-81.98322	
$2^{3}P_1$	-80.46223	
$3^{3}P_1$	-75.12151	
$4^{3}P_1$	-73.29433	
$5^{3}P_{4}$	-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 α^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 0.03×10^{-6} . Thus an α^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'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^{35,41,42} 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 $2^{3}P$ state.

Table VI presents relativistic contributions, to order α^2 , to the g factors of heliumlike ions from Li II to Ne IX. Matrix elements calculated by Pekeris⁴² were used in the application of Eq. (4.27) .

APPENDIX: EXPANSION OF POWERS OF THE INTERELECTRON DISTANCE

The expansion of powers of the interelectron The expansion of powers of the interelectron
distance r_{12} was discussed by Sack.³³ The series

$$
r_{12}^{-1} = r_2^{-1} \sum_{l=0}^{\infty} \left(\frac{r_2}{r_2}\right)^l P_l(\cos \theta_{12}), \tag{A1}
$$

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

	$2^{3}P_{1}$	$3^{3}P.$	4^3P	5^3P .
Li ⁷ \mathbf{u}	-187.52129	-171.9165	-166.548	-164.084
$Be9$ III	-338.8803	-308.136	-297.51	-292.6
R^{11} IV	-534.5915	-483.795	-466.19	-458.1
C^{12} v	-774.6687	-698.897	-672.59	-660.47
N^{14} VI	-1059.117	-953.44	-916.7	-899.77
Ω^{16} VII	-1387.938	-1247.43	-1198.6	-1176.0
F^{19} VIII	-1761.134	$-1580,871$	-1518.1	-1489.1
Ne^{20} JX	-2178.705	-1953.752	-1875.39	-1839.2

is well known. Jen⁴³ gave the expansion for r_{12} in terms of Legendre polynomials:

$$
r_{12} = r_2 \sum_{l=0}^{\infty} \left[\left(\frac{r_1}{r_2} \right)^2 \frac{1}{2l+3} - \frac{1}{2l-1} \right] \left(\frac{r_1}{r_2} \right)^l P_l(\cos \theta_{12})
$$
\n(A2)

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

$$
r_{12}^n = \sum_{i=0}^{\infty} R_{ni}(r_1, r_2) P_i(\cos \theta_{12}).
$$
 (A3)

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

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

where

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

The R_{nl} are given by:

$$
R_{nl}(r_1, r_2) = \frac{(-\frac{1}{2}n)_l}{(\frac{1}{2})_l} r_2^n \left(\frac{r_2}{r_2}\right)^l
$$

× $F(l - \frac{1}{2}n, -\frac{1}{2} - \frac{1}{2}n; l + \frac{3}{2}, r^2/r_2^n$). (A5)

The hypergeometric functions (A4} are finite series if either α or β is a negative integer or zero. Thus r_{12}^n can be expanded in a polynomial in $(r₅/r₅)^t$ 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 (Al) and (A2) we may explicitly write

$$
r_{12}^3 = 3r_5^3 \sum_{l} \left(\frac{r_5}{r_2}\right)^l \left(\left[(2l-1)(2l-3)\right]^{-1} - 2\left[(2l-1)(2l+3)\right]^{-1} \left(\frac{r_5}{r_2}\right)^2 + \left[(2l+3)(2l+5)\right]^{-1} \left(\frac{r_5}{r_2}\right)^4\right) P_l(\cos\theta_{12}), \quad \text{(A6)}
$$
\n
$$
r_{12}^5 = -15r_5^5 \sum_{l} \left(\frac{r_5}{r_2}\right)^l \left(\left[(2l-5)(2l-3)(2l-1)\right]^{-1} - 3\left[(2l-3)(2l-1)(2l+3)\right]^{-1} \left(\frac{r_5}{r_2}\right)^2 + 3\left[(2l-1)(2l+3)(2l+5)\right]^{-1} \left(\frac{r_5}{r_2}\right)^4 - \left[(2l+3)(2l+5)(2l+7)\right]^{-1} \left(\frac{r_5}{r_2}\right)^6\right) P_l(\cos\theta_{12}), \quad \text{(A7)}
$$

$$
r_{12}^7 = 105r_5^7 \sum_{l} \left(\frac{r_5}{r_5}\right)^l \left(\left[(2l-7)(2l-5)(2l-3)(2l-1)\right]^{-1} - 4\left[(2l-5)(2l-3)(2l-1)(2l+3)\right]^{-1} \left(\frac{r_5}{r_5}\right)^2 + 6\left[(2l-3)(2l-1)(2l+3)(2l+5)\right]^{-1} \left(\frac{r_5}{r_5}\right)^4 - 4\left[(2l-1)(2l+3)(2l+5)(2l+7)\right]^{-1} \left(\frac{r_5}{r_5}\right)^6 + \left[(2l+3)(2l+5)(2l+7)(2l+9)\right]^{-1} \left(\frac{r_5}{r_5}\right)^8 \right) P_l(\cos\theta_{12}), \tag{A8}
$$

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

$$
r_{12}^{-5} = \frac{1}{3(r_2^2 - r_1^2)^3} \sum_{l} \frac{r_1^l}{r_2^{l+1}} (2l+1) [(2l+3)r_2^2 - (2l-1)r_1^2] P_l(\cos\theta_{12}).
$$
 (A10)

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

$$
r_{12}^{-2} = \frac{1}{2r_1 r_2} \ln \frac{(r_1 + r_2)}{|r_1 - r_2|} + \left[\frac{3}{4} \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \ln \frac{(r_1 + r_2)}{|r_1 - r_2|} - \frac{3}{2r_1 r_2} \right] \cos \theta_{12} + \cdots
$$
 (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 (He, $2^3S_1/g_J$ (H, $1^2S_{1/2}$) has recently been reported [E. Aygün, B. D. Zak, and H. A. Shugart, Phys. Rev. Lett. 31, 803 (1973)i:

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

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

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- ~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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