High-precision calculations of the Zeeman effect in the 2 3PJ, 2 1P1, 2 3S1, and 3 3PJ states of helium

Z. C. Yan

Gordon W. F. Drake

University of Windsor
High-precision calculations of the Zeeman effect in the $2\,^3P_J$, $2\,^1P_1$, $2\,^3S_1$, and $3\,^3P_J$ states of helium

Zong-Chao Yan and G. W. F. Drake

Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4
(Received 1 June 1994)

The $g$ factors for the Zeeman effect, including relativistic corrections up to order $\alpha^2$ a.u., are calculated to high precision for the $2\,^3P_J$, $2\,^1P_1$, $2\,^3S_1$, and $3\,^3P_J$ states of helium, using variational wave functions constructed from doubled Hylleraas-type basis sets. Our results clarify the present disagreements among the existing theoretical values for the $g$ factors. The experimental values of the fine-structure splittings for the helium $3\,^3P_J$ states, measured by Yang et al. [Phys. Rev. A 32, 2249 (1985); 33, 1725 (1986)], are reanalyzed, using our improved $g$ factors.

PACS number(s): 31.20.Di, 31.30.Jv

I. INTRODUCTION

The Zeeman effect in helium provides a fundamental testing ground for the theory of atomic interactions with external fields. If the theory of the Zeeman effect is sufficiently well understood, then it can be used to extract high-precision values for the fine-structure splittings of triplet states at zero magnetic field strength from the measured locations of field-induced level crossings [1]. However, there is a long-standing discrepancy between theory and experiment for the Zeeman coupling factor $g_I'$ for the $2\,^3P$ state of helium, even when relativistic corrections of $O(\alpha^2)$ are included [2].

In an effort to resolve this discrepancy, Anthony and Sebastian [2] have recently recalculated the Zeeman $g$ factors, using a 125-term configuration-interaction wave function and including the next-higher-order terms of $O(\alpha^3)$ and $O(\alpha^2 m_J/M_{He})$. Although the higher-order terms are too small to account for the discrepancy, their $g$ factors are not in good agreement with the previous values of Lewis and Hughes [3].

The present paper has two main objectives. The first is to perform definitive high-precision calculations of the Zeeman $g$ factors in order to resolve the differences among existing calculations. The second is to reanalyze the magnetic-field level-crossing measurements of Yang and co-workers [1] in order to obtain improved values for the fine-structure splittings of the helium $3\,^3P$ state. Since their experimental error was dominated by uncertainties due to $g$ factors calculated from hydrogenic wave functions, we are able to decrease the uncertainties by about a factor of 2 for the intervals $v_{01}$ and $v_{12}$.

II. THEORY

The Zeeman Hamiltonian, including relativistic corrections of $O(\alpha^2)$, was derived from the Breit interaction by Perl and Hughes [4] and by Van Vleck and co-workers [5,6]. Detailed descriptions of the evaluation of the various terms with correlated Hylleraas wave functions have been given by Lewis, Pichanick, and Hughes [7] and Lewis and Hughes [3]. The terms to be evaluated are briefly summarized in this section.

We adopt the $LS$ coupling scheme in our calculation. Using standard angular momentum theory [8], the expectation value of the Zeeman Hamiltonian becomes

$$
\langle LSJ'M_J|H_{\text{Zeeman}}|LSJM_J\rangle = \langle \mu_B H \rangle (-1)^{1-M_J(J',J')} \left[ \begin{array}{c} J' & 1 & J \\ -M_J & 0 & M_J \end{array} \right] \sqrt{6} \left[ \begin{array}{c} L & J' & S \\ J & L & 1 \end{array} \right] (-1)^{l'+J'+L+S} g_L' + \left[ \begin{array}{c} J & 1 \\ S & L \\ S' & \end{array} \right] \langle -1 \rangle^{L+S} g_s' + (-1)^{J'} \left[ \begin{array}{c} L & 2 \\ S & 1 \\ J & 1 \end{array} \right] g_s.
$$

$$
+ \frac{2}{3} \langle \mu_B H \rangle (-1)^{J'+J'-M_J(J',J')} \left[ \begin{array}{c} J' & 0 & J \\ -M_J & 0 & M_J \end{array} \right] \left[ \begin{array}{c} L & J' & S \\ J & L & 0 \end{array} \right] (-1)^{L+S} g_{Q1}
$$

$$
- \left[ \begin{array}{c} J' & 2 \\ -M_J & 0 & M_J \end{array} \right] \left[ \begin{array}{c} L & J' & S \\ J & L & 2 \end{array} \right] (-1)^{L+S} g_{Q2}.
$$

(1)

where $(\alpha,\beta,\ldots)=(2\alpha+1)(2\beta+1)\ldots$, $H$ is the external magnetic field, and $\mu_B$ is the Bohr magneton. The five $g$ factors, which characterize the Zeeman effect to order $\alpha^2$, can be further expressed in terms of 11 reduced matrix elements according to

$$
1050 \rightarrow 2947/94/50(3)/1980(4)/$06.00

50 R1980 © 1994 The American Physical Society
TABLE I. Convergence study of the reduced matrix element $F_4$ for the $2\,^{3}P_J$ states of helium (in arbitrary units). $N$ is the number of terms in the basis set.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$F_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>104</td>
<td>1.530 869 811 933</td>
</tr>
<tr>
<td>145</td>
<td>1.530 940 828 474</td>
</tr>
<tr>
<td>197</td>
<td>1.530 954 527 354</td>
</tr>
<tr>
<td>264</td>
<td>1.530 965 591 545</td>
</tr>
<tr>
<td>342</td>
<td>1.530 965 977 252</td>
</tr>
<tr>
<td>436</td>
<td>1.530 965 973 542</td>
</tr>
<tr>
<td>539</td>
<td>1.530 965 970 190</td>
</tr>
<tr>
<td>658</td>
<td>1.530 965 962 219</td>
</tr>
<tr>
<td>724</td>
<td>1.530 965 959 591</td>
</tr>
<tr>
<td>804</td>
<td>1.530 965 962 630</td>
</tr>
<tr>
<td>Extrapolation</td>
<td>1.530 965 962 615(32)</td>
</tr>
</tbody>
</table>

\[
g'_L = \frac{\sqrt{(2L+1)(L+1)}}{6} g_L + \frac{2\,m}{\sqrt{6\,M}} F_1 + a^2 \frac{1}{\sqrt{6}} (F_2 + F_3 - F_4),
\]

\[
g'_g = \frac{\sqrt{(2S+1)(S+1)}}{6} g_g + a^2 (-1)^S \frac{(2S+1)}{2L+1} \times \left\{ \begin{array}{c}
\frac{1}{2} S \\
\frac{1}{2} \end{array} \right\} \left\{ \begin{array}{c}
F_s + \frac{Z}{3} F_6 - \frac{1}{2} F_7 \\
S + \frac{1}{2} \end{array} \right\},
\]

\[
g_s = a^2 (-1)^S \left( 2S+1 \right) \left\{ \begin{array}{c}
\frac{1}{2} S \\
\frac{1}{2} \end{array} \right\} \sqrt{\frac{\hbar^2}{6}} \left( -ZF_8 + \frac{5}{2} F_9 \right),
\]

TABLE II. Reduced matrix elements $F_i$ for $2\,^{3}P_J$, $3\,^{3}P_J$, $2\,^{1}P_J$, and $2\,^{3}S_J$ states of helium. $F_i^{(0)}$ is the matrix element without the mass polarization and mass scaling, $F_i^{MP}$ is the correction due to the mass polarization, and $F_i^{MS}$ is the correction due to the mass scaling. Units are atomic units.

<table>
<thead>
<tr>
<th>Term</th>
<th>$F_i^{(0)}$</th>
<th>$10^6 F_i^{MP}$</th>
<th>$10^6 F_i^{MS}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_1$</td>
<td>0.157 303 736 2(12)</td>
<td>202.168 5(12)</td>
<td>0</td>
</tr>
<tr>
<td>$F_2$</td>
<td>0.064 656 953 490 1(61)</td>
<td>63.081 767(14)</td>
<td>-8.871 471(18)</td>
</tr>
<tr>
<td>$F_3$</td>
<td>-0.385 703 681 446 57(95)</td>
<td>-88.843 615 5(13)</td>
<td>105.757 434(2)</td>
</tr>
<tr>
<td>$F_4$</td>
<td>-0.003 061 931 925 238(73)</td>
<td>-2.384 469 81(20)</td>
<td>0.420 039 83(27)</td>
</tr>
<tr>
<td>$F_5$</td>
<td>-3.694 748 759 315 750(98)</td>
<td>-30.681 595 77(13)</td>
<td>1 012.851 126 58(11)</td>
</tr>
<tr>
<td>$F_6$</td>
<td>1.962 833 452 601 313(35)</td>
<td>18.579 979 726(45)</td>
<td>-269.057 083 311(40)</td>
</tr>
<tr>
<td>$F_7$</td>
<td>0.461 836 293 613 323(48)</td>
<td>43.644 994 260(68)</td>
<td>-63.311 990 425(67)</td>
</tr>
<tr>
<td>$F_8$</td>
<td>-0.153 723 698 780(19)</td>
<td>-15.874 753(28)</td>
<td>21.073 785(30)</td>
</tr>
<tr>
<td>$F_9$</td>
<td>-0.278 910 517 473 78(58)</td>
<td>-29.744 339 89(82)</td>
<td>38.235 614 30(81)</td>
</tr>
<tr>
<td>$F_{10}$</td>
<td>22.883 405 929 55(20)</td>
<td>-3 543.981 48(29)</td>
<td>6 273.784 06(29)</td>
</tr>
<tr>
<td>$F_{11}$</td>
<td>-14.055 466 357 05(12)</td>
<td>2 253.696 31(18)</td>
<td>-3 853.468 25(19)</td>
</tr>
<tr>
<td>$F_1$</td>
<td>0.042 717 180 72(30)</td>
<td>172.135 77(38)</td>
<td>0</td>
</tr>
<tr>
<td>$F_2$</td>
<td>0.018 790 495 776 86(7)</td>
<td>22.596 849(11)</td>
<td>-2.578 796(12)</td>
</tr>
<tr>
<td>$F_3$</td>
<td>-0.159 197 889 073 43(11)</td>
<td>-21.498 375 08(15)</td>
<td>43.646 864(05)</td>
</tr>
<tr>
<td>$F_4$</td>
<td>-0.001 051 388 333 38(18)</td>
<td>-0.434 316 60(18)</td>
<td>0.144 178 129(57)</td>
</tr>
<tr>
<td>$F_5$</td>
<td>-3.564 701 004 060 508 3(69)</td>
<td>-8.729 204 528(16)</td>
<td>977.195 074 026(21)</td>
</tr>
<tr>
<td>$F_6$</td>
<td>1.832 549 223 716 723(19)</td>
<td>4.928 816 090(36)</td>
<td>-251.196 558 370(42)</td>
</tr>
<tr>
<td>$F_7$</td>
<td>0.200 794 886 747 011(46)</td>
<td>10.988 347 504(62)</td>
<td>-27.525 377 438(59)</td>
</tr>
<tr>
<td>$F_8$</td>
<td>-0.065 818 327 340(70)</td>
<td>-3.771 40(10)</td>
<td>9.022 54(10)</td>
</tr>
<tr>
<td>$F_9$</td>
<td>-0.124 105 227 572 44(23)</td>
<td>-7.672 052 97(34)</td>
<td>17.012 721 39(35)</td>
</tr>
<tr>
<td>$F_{10}$</td>
<td>142.218 504 711 9(12)</td>
<td>-12 988.601 5(17)</td>
<td>38 993.535 1(16)</td>
</tr>
<tr>
<td>$F_{11}$</td>
<td>-89.534 381 547 46(79)</td>
<td>8 217.626 8(11)</td>
<td>-24 548.566 8(10)</td>
</tr>
</tbody>
</table>

$2\,^{3}P_J$, $3\,^{3}P_J$, $2\,^{1}P_J$, $2\,^{3}S_J$
TABLE III. Comparison of theoretical and experimental g factors for the \( 2 \, ^3P_J \), \( 2 \, ^1P_1 \), \( 2 \, ^3S_1 \) and \( 3 \, ^3P_J \) states of helium. Here \( m/M = 1.370 \times 10^{-4} \), \( \alpha^{-1} = 137.035 \times 10^5 \) cm \( ^{-1} \), \( R_m = 109.737 \times 10^8 \) cm \( ^{-1} \), and \( c = 2.997 \times 10^{10} \) cm sec \( ^{-1} \). The errors quoted in our g factors do not include the errors in the fundamental constants.

<table>
<thead>
<tr>
<th>Present work</th>
<th>Previous work</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^6 \delta g_L )</td>
<td>[ \begin{align*} 10.719 \times 10^9 &amp; \quad (19) \ -80.436 \times 10^4 &amp; \quad 6(38) \ -5.391 \times 10^5 &amp; \quad 9(21) \end{align*} ]</td>
<td>[ \begin{align*} -80.46(1)^a &amp; \quad 80.401^b \quad -76.0(2.4)^d \ -3.5(2.5)^a &amp; \quad -5.344^b &amp; \quad 4.0(25.0)^d \end{align*} ]</td>
</tr>
<tr>
<td>( g_{Q1} )</td>
<td>[ \begin{align*} 22.886 &amp; \quad 135 \quad 732 \quad 12(20) \ -14.057 &amp; \quad 066 \quad 129 \quad 01(13) \end{align*} ]</td>
<td>[ \begin{align*} 22.54 &amp; \quad 135 \quad 732 \quad 12(20) \ -14.057 &amp; \quad 066 \quad 129 \quad 01(13) \end{align*} ]</td>
</tr>
<tr>
<td>( \delta g_S )</td>
<td>[ \begin{align*} -81.956 &amp; \quad 037 \quad 002 \quad 152(17) \ 11.467 &amp; \quad 588 \quad 230 \quad 724 \quad 521(12) \end{align*} ]</td>
<td>[ \begin{align*} -81.983 &amp; \quad 22 \quad 152(17) \ 11.467 &amp; \quad 588 \quad 230 \quad 724 \quad 521(12) \end{align*} ]</td>
</tr>
</tbody>
</table>

\( ^a \) Lewis and Hughes [3].
\( ^b \) Anthony and Sebastian [2].
\( ^c \) Lhuillier et al. [12].
\( ^d \) Lewis et al. [7].
\( ^e \) Kramer and Pipkin [11].

\[
\begin{align*}
\delta Q_1 &= F_{10}, \\
\delta Q_2 &= F_{11},
\end{align*}
\]

where

\[
g_L = 1 - m/M,
\]

\[
g_S = 2 \left[ 1 + \alpha/2 \pi - 0.328 \times 10^{-2} \alpha^2 \right],
\]

\( m/M \) is the electron to nuclear mass ratio, and \( Z \) is the atomic number. The reduced matrix elements \( F_i \) are defined by

\[
F_1 = \langle L \parallel i \parallel (r_1 \times \nabla_2) \parallel L \rangle,
\]

\[
F_2 = \langle L \parallel i \parallel (1/r_{12}) \parallel (r_1 \times \nabla_2) \parallel L \rangle,
\]

\[
F_3 = \langle L \parallel -i \nabla_1^2 (1/r_1 \times \nabla_1) \parallel L \rangle,
\]

\[
F_4 = \langle L \parallel i \parallel (1/r_{12}) \parallel (r_1 \times r_2) \parallel (r_{12} \times \nabla_2) \parallel L \rangle,
\]

\[
F_5 = \langle L \parallel \nabla_1^2 \parallel L \rangle,
\]

\[
F_6 = \langle L \parallel 1/r_1 \parallel L \rangle,
\]

\[
F_7 = \langle L \parallel 1/r_{12} \parallel L \rangle,
\]

\[
F_8 = \langle L \parallel (1/r_1) C_2(\tilde{r}_1) \parallel L \rangle,
\]

\[
F_9 = \langle L \parallel (1/r_{12}) C_2(\tilde{r}_{12}) \parallel L \rangle,
\]

\[
F_{10} = \langle L \parallel r_1^2 \parallel L \rangle,
\]

\[
F_{11} = \langle L \parallel r_1^2 C_2(\tilde{r}_1) \parallel L \rangle,
\]

where \( C_k^\ell \) is related to the spherical harmonics by

\[
C_k^\ell = \sqrt{4\pi/(2k+1)} Y_k^\ell (\hat{r})
\]

and \( r_{12} = r_1 - r_2 \).

### III. CALCULATIONS AND RESULTS

The necessary matrix elements in Eqs. (9)–(19) were calculated to high precision by the use of variational wave functions constructed from doubled basis sets in Hylleraas coordinates, as described previously [9]. The explicit form for the wave functions is

\[
\Psi(r_1, r_2) = \sum_{ijk} [a_{ij}^{(1)} \chi_{ij}^{(k)}(\alpha_1, \beta_1) + a_{ij}^{(2)} \chi_{ij}^{(k)}(\alpha_2, \beta_2)]
\]

\times (\text{angular function}) \pm (\text{exchange}),

with

**TABLE IV.** Experimental values of the fine-structure splittings for the \( 3 \, ^3P_J \) states of helium. Units are MHz.

<table>
<thead>
<tr>
<th>Interval</th>
<th>Present work</th>
<th>Previous work [1]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nu_1 )</td>
<td>8.113.965(38) (4.7 ppm)</td>
<td>8.113.969(80) (9.8 ppm)</td>
</tr>
<tr>
<td>( \nu_{12} )</td>
<td>658.561(36) (55 ppm)</td>
<td>658.548(69) (105 ppm)</td>
</tr>
<tr>
<td>( \nu_{102} )</td>
<td>8.772.526(13) (1.5 ppm)</td>
<td>8.772.517(16) (1.9 ppm)</td>
</tr>
</tbody>
</table>
\[ X_{ijk} = r_i r_j^k e^{-ar_1 - br_2} \]

and \( i + j + k \leq \Omega \). A complete optimization is then performed with respect to the two sets of nonlinear parameters \( \alpha_1, \beta_1 \) and \( \alpha_2, \beta_2 \). The screened hydrogenic wave function is also included explicitly in the basis set. These techniques yield much improved convergence relative to single basis-set calculations.

Each of the \( F_i \) matrix elements is first evaluated with respect to wave functions which satisfy the Schrödinger equation for infinite nuclear mass. To a first approximation, finite mass corrections come from the mass scaling of distances according to \( r \rightarrow (m/M)r \), where \( \mu = mM/(m + M) \) is the reduced mass, and from the perturbative effect of including the \( -(\mu/M)\nabla_1 \cdot \nabla_2 \) mass polarization term in the Hamiltonian.

A typical convergence study with the size of the basis set is shown in Table I for \( F_{14} \). Table II lists all the nonvanishing reduced matrix elements \( F_i \) for the \( 2^3P_j, 3^3P_j, 2^1P_1 \), and \( 2^3S_1 \) states of helium. The final \( g \) values are shown in Table III, together with the existing theoretical and experimental values. The results are expressed in terms of the quantities \( \delta g_L \) and \( \delta g_S \) defined by

\[ \delta g_L = g'_L - \sqrt{(2L + 1)L(L + 1)/6} \ g_L, \]
\[ \delta g_S = g'_S - \sqrt{(2S + 1)S(S + 1)/6} \ g_S. \]

Our results for the \( g'_L \) and \( g'_S \) agree with but are much more accurate than those of Lewis and Hughes [3,10]. However, our results for \( g'_L \) differ substantially from those of Anthony and Sebastian [2], especially for the \( 2^3P_J \) and \( 2^1P_1 \) states. This is likely due to the slow convergence of their configuration-interaction calculation. The values for \( g'_S \) and \( g_x \) are in reasonable agreement. The \( g_{Q1} \) and \( g_{Q2} \) values for the \( 2^3P_J \) states of Lewis et al. [7] were calculated using hydrogenic wave functions. Their notations for \( R_{14} \) and \( R_{15} \) are related to \( g_{Q1} \) and \( g_{Q2} \) by

\[ g_{Q1} = \sqrt{3}/2 \ (R_{14} + R_{15}), \]
\[ g_{Q2} = -\sqrt{3}/10 \ R_{15}. \]

for the \( 3^3P_J \) states. Our theoretical values for \( g'_L \) and \( g'_S \) are within two standard deviations of the experimental errors. For \( g_x \), our value is within one standard deviation, but here the experimental uncertainty is large. The discrepancies between theory and experiment are too large to be significantly changed by including next-higher-order relativistic corrections to the Zeeman effect, as calculated by Anthony and Sebastian [2]. Improved measurements would be of considerable interest.

Recently, Yang and co-workers [1] reported high-precision measurements of the magnetic fields at the crossing points between the \( (J,M_J)=(0,0) \) and \( (2,2) \), and the \( (J,M_J)=(0,0) \) and \( (1,1) \) sublevels in the \( 3^3P_J \) states of helium. In order to obtain the fine-structure splittings, they used the Zeeman \( g \) factors which were calculated by Kramer and Pipkin [11] from hydrogenic wave functions. As noted by Yang and co-workers, their accuracy was limited by their theoretical uncertainties in the Zeeman effect calculation. We have reanalyzed their experimental results, using our improved Zeeman \( g \) factors. The fine-structure splittings thus obtained are listed in Table IV. The uncertainties in the revised values of 8113.965(38) and 658.561(36) MHz for \( \nu_0 \) and \( \nu_{12} \), respectively, have been reduced by about a factor of 2.

**IV. CONCLUSIONS**

A high-precision calculation has been performed for the lowest-order \( \alpha^2 \) relativistic correction to the Zeeman effect in the \( 2^3P_J, 3^3P_J, 2^1P_1 \), and \( 3^3P_J \) states of helium. Our results provide precise values for the \( g \) factors. Application of our results to the \( 3^3P_J \) fine structure of helium has led to an improved determination of the experimental fine-structure intervals. Comparisons with theoretical values of the fine-structure intervals up to terms of \( O(\alpha^6m^2c^2) \) will be presented in a future publication. However, the disagreement between the theoretical and experimental \( g \) factors, especially the \( g'_L \) factor for the \( 3^3P_J \) state, still persists.

**ACKNOWLEDGMENT**

Research support by the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

---