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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

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The g factors for the Zeeman effect, including relativistic corrections up to order α^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.

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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_L' 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 $O(\alpha^2 m_e/M_{\rm He})$. 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 ν_{01} and ν_{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

$$\begin{aligned}\langle LSJ'M_J|H_{\rm Zeeman}|LSJM_J\rangle=(\mu_B H)(-1)^{1-M_J}(J,J')^{1/2}\begin{pmatrix} J' & 1 & J \\ -M_J & 0 & M_J\end{pmatrix}\sqrt{6}\Bigg[\begin{Bmatrix} L & J' & S \\ J & L & 1\end{Bmatrix}(-1)^{J+J'+L+S}g_L' \\ +\begin{Bmatrix} J & J' & 1 \\ S & S & L\end{Bmatrix}(-1)^{L+S}g_S'+(-1)^{J'}\begin{Bmatrix} L & L & 2 \\ S & S & 1 \\ J' & J & 1\end{Bmatrix}g_x\Bigg] \\ +\frac{2}{3}(\mu_B H)^2(-1)^{J+J'-M_J}(J,J')^{1/2}\Bigg[\begin{pmatrix} J' & 0 & J \\ -M_J & 0 & M_J\end{pmatrix}\begin{Bmatrix} L & J' & S \\ J & L & 0\end{Bmatrix}(-1)^{L+S}g_{Q1} \\ -\begin{pmatrix} J' & 2 & J \\ -M_J & 0 & M_J\end{pmatrix}\begin{Bmatrix} L & J' & S \\ J & L & 2\end{Bmatrix}(-1)^{L+S}g_{Q2}\Bigg]\,, \end{aligned} \tag{1}$$

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

TABLE I. Convergence study of the reduced matrix element F_4 for the $2\ ^3P_J$ states of helium (in arbitrary units). N is the number of terms in the basis set.

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

$$g_L' = \sqrt{\frac{(2L+1)L(L+1)}{6}}\, g_L + \frac{2}{\sqrt{6}}\frac{m}{M} F_1 + \alpha^2 \frac{1}{\sqrt{6}} (F_2 + F_3 - F_4), \tag{2}$$

$$g_S' = \sqrt{\frac{(2S+1)S(S+1)}{6}}\, g_S + \alpha^2 (-1)^S \frac{(2S+1)}{\sqrt{2L+1}} \times \begin{Bmatrix} \frac{1}{2} & S & \frac{1}{2} \\ S & \frac{1}{2} & 1 \end{Bmatrix} \left(F_5 + \frac{Z}{3} F_6 - \frac{1}{2} F_7 \right), \tag{3}$$

$$g_x = \alpha^2 (-1)^S (2S+1) \begin{Bmatrix} \frac{1}{2} & S & \frac{1}{2} \\ S & \frac{1}{2} & 1 \end{Bmatrix} \sqrt{\tfrac{5}{6}}\, (-ZF_8 + \tfrac{3}{2} F_9), \tag{4}$$

TABLE II. Reduced matrix elements F_i for $2\ ^3P_J$, $3\ ^3P_J$, $2\ ^1P_1$, and $2\ ^3S_1$ 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.

Term	$F_i^{(0)}$	$10^6\, F_i^{\mathrm{MP}}$	$10^6\, F_i^{\mathrm{MS}}$
		$2\ ^3P_J$	
F_1	0.157 303 736 2(12)	202.168 5(12)	0
F_2	0.064 656 953 490 1(61)	63.081 767(14)	−8.871 471(18)
F_3	−0.385 703 681 446 57(95)	−88.843 615 5(13)	105.757 434 2(14)
F_4	−0.003 061 931 925 238(73)	−2.384 469 81(20)	0.420 039 83(27)
F_5	−3.694 748 759 315 750(98)	−30.681 595 77(13)	1 012.851 126 58(11)
F_6	1.962 833 453 061 313(35)	18.579 979 726(45)	−269.057 083 311(40)
F_7	0.461 836 293 613 323(48)	43.644 994 260(68)	−63.311 990 425(67)
F_8	−0.153 723 698 780(19)	−15.874 753(28)	21.073 785(30)
F_9	−0.278 910 517 473 78(58)	−29.744 339 89(82)	38.235 614 30(81)
F_{10}	22.883 405 929 55(20)	−3 543.981 48(29)	6 273.784 06(29)
F_{11}	−14.055 466 357 07(12)	2 253.696 31(18)	−3 853.468 25(19)
		$3\ ^3P_J$	
F_1	0.042 717 180 72(30)	172.135 77(38)	0
F_2	0.018 790 495 776 8(67)	22.596 849(11)	−2.578 796(12)
F_3	−0.159 197 889 073 43(11)	−21.498 375 08(15)	43.646 864 05(15)
F_4	−0.001 051 388 333 38(18)	−0.434 318 60(18)	0.144 178 129 7(57)
F_5	−3.564 701 004 060 508 3(69)	−8.729 204 528(16)	977.195 074 026(21)
F_6	1.832 549 223 716 723(19)	4.928 816 090(36)	−251.196 558 370(42)
F_7	0.200 794 886 747 011(46)	10.988 347 504(62)	−27.525 377 438(59)
F_8	−0.065 818 327 340(70)	−3.771 40(10)	9.022 54(10)
F_9	−0.124 105 227 572 44(23)	−7.672 052 97(34)	17.012 721 39(35)
F_{10}	142.218 504 711 9(12)	−12 988.601 5(17)	38 993.535 1(16)
F_{11}	−89.534 381 547 46(79)	8 217.626 8(11)	−24 548.566 8(10)
		$2\ ^1P_1$	
F_1	−0.080 247 745 85(29)	189.930 6(19)	0
F_2	−0.047 158 325 902(16)	54.958 489(95)	6.456 67(13)
F_3	−0.295 788 312 262 9(12)	50.227 028 2(20)	81.070 780 4(23)
F_4	0.018 289 571 230 2(12)	−7.229 844 4(17)	−2.506 043 9(16)
F_{10}	27.306 915 372 95(84)	3 347.265 3(12)	7 488.624 3(12)
F_{11}	−16.854 584 168 39(54)	−2 126.688 01(76)	−4 622.202 88(76)
		$2\ ^3S_1$	
F_5	−2.175 229 378 236 790 63(22)	2.037 012 682 76(31)	596.295 800 158 829(31)
F_6	1.154 664 152 972 106 89(22)	−0.661 597 944 10(25)	−158.274 992 697 17(16)
F_7	0.268 197 855 414 847 586(28)	−0.608 298 794 890(39)	−36.763 020 261 598(39)
F_{10}	11.464 321 622 284 606(36)	122.994 634 436(38)	3 143.613 805 479(18)

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 $m/M=1.370\,933\,543\times10^{-4}$, $\alpha^{-1}=137.035\,989\,5(61)$, $R_\infty=109\,737.315\,709(18)$ cm^{-1}, and $c=2.997\,924\,58\times10^{10}$ cm sec^{-1}. The errors quoted in our g factors do not include the errors in the fundamental constants.

	Present work	Previous work		Experiment
		$2\,^3P_J$		
$10^6\delta g_L$	10.719 291 348 (19)	10.6(4)[a]	8.838[b]	4.9(2.9)[c]
$10^6\delta g_S$	−80.436 904 988 692 6(38)	−80.46(1)[a]	−80.401[b]	−76.0(2.4)[d]
$10^6 g_x$	−5.391 808 409 9(21)	−3.5(2.5)[a]	−5.344[b]	4.0(25.0)[d]
g_{Q1}	22.886 135 732 12(20)	22.5[d]		
g_{Q2}	−14.057 066 129 01(13)	−13.8[d]		
		$2\,^1P_1$		
$10^6\delta g_L$	−16.810 165 65(21)		−15.771[b]	
g_{Q1}	27.317 751 262 54(84)			
g_{Q2}	−16.861 333 059 28(54)			
		$2\,^3S_1$		
$10^6\delta g_S$	−81.956 037 002 663 152(17)	−81.983 22[a]		
g_{Q1}	11.467 588 230 724 521(12)			
		$3\,^3P_J$		
$10^6\delta g_L$	1.772 223 929(26)	−0.17(2.8)[e]		
$10^6\delta g_S$	−75.096 557 468 968 2(17)	−75.13(3.27)[e]	−75.121 51[a]	
$10^6 g_x$	−2.650 192 659 3(71)	−2.75(10.02)[e]		
g_{Q1}	142.244 509 645 5(11)	137.21[e]		
g_{Q2}	−89.550 712 487 54(72)	−86.37[e]		

[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].

$$g_{Q1}=F_{10}, \tag{5}$$

$$g_{Q2}=F_{11}, \tag{6}$$

where

$$g_L=1-m/M, \tag{7}$$

$$g_S=2\,[1+\alpha/2\pi-0.328\,478\,965(\alpha^2/\pi^2)+\cdots]\,, \tag{8}$$

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

$$F_1=\langle L\|i(\mathbf{r}_1\times\nabla_2)\|L\rangle, \tag{9}$$

$$F_2=\langle L\|i(1/r_{12})(\mathbf{r}_1\times\nabla_2)\|L\rangle, \tag{10}$$

$$F_3=\langle L\|-i\nabla_1^2(\mathbf{r}_1\times\nabla_1)\|L\rangle, \tag{11}$$

$$F_4=\langle L\|i(1/r_{12}^3)(\mathbf{r}_1\times\mathbf{r}_2)(\mathbf{r}_{12}\cdot\nabla_2)\|L\rangle, \tag{12}$$

$$F_5=\langle L\|\nabla_1^2\|L\rangle, \tag{13}$$

$$F_6=\langle L\|1/r_1\|L\rangle, \tag{14}$$

$$F_7=\langle L\|1/r_{12}\|L\rangle, \tag{15}$$

$$F_8=\langle L\|(1/r_1)C_2(\hat{\mathbf{r}}_1)\|L\rangle, \tag{16}$$

$$F_9=\langle L\|(1/r_{12})C_2(\hat{\mathbf{r}}_{12})\|L\rangle, \tag{17}$$

$$F_{10}=\langle L\|r_1^2\|L\rangle, \tag{18}$$

$$F_{11}=\langle L\|r_1^2C_2(\hat{\mathbf{r}}_1)\|L\rangle, \tag{19}$$

where C_k^q is related to the spherical harmonics by $C_k^q=\sqrt{4\pi/(2k+1)}Y_k^q(\hat{\mathbf{r}})$ and $\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2$.

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

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\sum_{ijk}\,[a_{ijk}^{(1)}\chi_{ijk}(\alpha_1,\beta_1)+a_{ijk}^{(2)}\chi_{ijk}(\alpha_2,\beta_2)]$$
$$\times(\text{angular function})\pm(\text{exchange})\,, \tag{20}$$

with

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

Interval	Present work	Previous work [1]
ν_{01}	8 113.965(38) (4.7 ppm)	8 113.969(80) (9.8 ppm)
ν_{12}	658.561(36) (55 ppm)	658.548(69) (105 ppm)
ν_{02}	8 772.526(13) (1.5 ppm)	8 772.517(16) (1.9 ppm)

$$\chi_{ijk}=r_1^i r_2^j r_{12}^k e^{-\alpha r_1-\beta r_2} \tag{21}$$

and $i+j+k\leq\Omega$. A complete optimization is then performed with respect to the two sets of nonlinear parameters α_1,β_1 and α_2,β_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 $r\rightarrow(m/\mu)r$, 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_4. 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 δg_L and δg_S defined by

$$\delta g_L=g_L'-\sqrt{(2L+1)L(L+1)/6}\;g_L\,, \tag{22}$$

$$\delta g_S=g_S'-\sqrt{(2S+1)S(S+1)/6}\;g_S. \tag{23}$$

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

$$g_{Q1}=\sqrt{3}/2\;\;(R_{14}+R_{15}), \tag{24}$$

$$g_{Q2}=-\sqrt{3/10}\;\;R_{15} \tag{25}$$

for the ^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 ν_{01} and ν_{12}, respectively, have been reduced by about a factor of 2.

IV. CONCLUSIONS

A high-precision calculation has been performed for the lowest-order α^2 relativistic correction to the Zeeman effect in the $2\,^3P_J$, $2\,^1P_1$, $2\,^3S_1$ 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 $O(\alpha^6mc^2)$ will be presented in a future publication. However, the disagreement between the theoretical and experimental g factors, especially the g_L' factor for the $2\,^3P_J$ state, still persists.

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