Relativistic corrections to the Zeeman effect of lithium and lithiumlike ions in the $2\,^2P_J$ and $3\,^2P_J$ states

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The Zeeman g_J factors are calculated for the $2\,^2P_J$ and $3\,^2P_J$ states of lithium and lithiumlike ions, including relativistic corrections of order α^2, using variational wave functions in Hylleraas coordinates. Comparison with other calculations is made.

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I. INTRODUCTION

Recently we have performed several calculations [1–3] of the Zeeman g_J factors for lithium and its low-Z ions in S states. The formalism is based on the extended Breit equation of Hegstrom [4] which includes relativistic corrections of order α^2 a.u. (atomic units are used throughout), relativistic recoil corrections of order $\alpha^2 m/M$, and radiative corrections of order α^3. Although this theory was proven rigorously to be accurate up to α^3 for a neutral atomic system in an S state, it is expected that the extended Breit equation also describes the Zeeman effect accurately to order α^3 for an S-state low-Z ion. For non-S states, however, the theory is correct only to the order of α^2, although computationally it is much more demanding than the S-state case due to nonvanishing angular terms. So far, most of the calculations have concentrated on S states, except the work of Guan and Wang [5], who were the first to evaluate the relativistic corrections to the Zeeman g_J factors of lithium in the $n\,^2P_J$ states with n up to 5, using the method of full core plus correlation. Nevertheless, it is difficult to assess the reliability of their calculations (see the discussion in Sec. III). Since the values of g_J factors are important in high-precision measurements [6–9], it is desirable to calculate the g_J factors definitively using high-quality wave functions. For two-electron atomic systems, such work has been carried out by several authors, including Lewis and Hughes [10], Anthony and Sebastian [11], and Yan and Drake [12], who used the calculated g_J factors to reanalyze the level-crossing experimental values of the fine-structure splittings for the $3\,^3P_J$ states of helium measured by Yang *et al.* [6,7]. The main purpose of this paper is to present high-precision calculations of the g_J factors for lithium and lithiumlike ions in the $2\,^2P_J$ and $3\,^2P_J$ states, with Z up to 12, including relativistic corrections of order α^2. The second purpose is to establish a benchmark for other atomic structure calculations involving three electrons. It should be pointed out that, as the nuclear charge Z increases, the electron-nuclear interaction will eventually dominate electron-electron correlations, and thus higher-order relativistic and QED effects become important. At present, the theory of higher-order effects, however, is available only for one-electron hydrogenic systems [13].

II. FORMULATION

The starting point is the magnetic-field-dependent part of the Hamiltonian [4]

$$H_{\rm Zeeman}=\sum_{i=0}^{6} H_i, \tag{1}$$

where

$$H_0=\mu_B\mathbf{H}\cdot(g_L\mathbf{L}+g_S\mathbf{S}), \tag{2}$$

$$H_1=-\frac{1}{2}\alpha^2\mu_B\mathbf{H}\cdot\sum_j \nabla_j^2(i\mathbf{r}_j\times\boldsymbol{\nabla}_j)$$

$$+\alpha^2\mu_B\mathbf{H}\cdot\sum_j \mathbf{s}_j\nabla_j^2, \tag{3}$$

$$H_2=\frac{Z}{2}\alpha^2\mu_B\mathbf{H}\cdot\sum_j\left[\frac{2\mathbf{s}_j}{3r_j}+\frac{1}{3r_j}\left(\mathbf{s}_j-\frac{3\mathbf{r}_j(\mathbf{r}_j\cdot\mathbf{s}_j)}{r_j^2}\right)\right], \tag{4}$$

$$H_3=\frac{1}{2}\alpha^2\mu_B\mathbf{H}\cdot\sum_{j\neq k}\frac{1}{r_{jk}^3}[(\mathbf{s}_j+2\mathbf{s}_k)\times\mathbf{r}_{jk}]\times\mathbf{r}_j, \tag{5}$$

$$H_4=\frac{1}{2}\alpha^2\mu_B\mathbf{H}\cdot\sum_{k>j}\left[i\frac{1}{r_{jk}}(\mathbf{r}_j\times\boldsymbol{\nabla}_k+\mathbf{r}_k\times\boldsymbol{\nabla}_j)\right.$$

$$\left.-\frac{i}{r_{jk}^3}(\mathbf{r}_j\times\mathbf{r}_k)\mathbf{r}_{jk}\cdot(\boldsymbol{\nabla}_j+\boldsymbol{\nabla}_k)\right], \tag{6}$$

$$H_5=\frac{m}{M}\mu_B\mathbf{H}\cdot\sum_{j\neq k}(i\mathbf{r}_j\times\boldsymbol{\nabla}_k), \tag{7}$$

$$H_6=\frac{1}{3}(\mu_B H_Z)^2\sum_j r_j^2[1-C_2^0(\mathbf{r}_j)]. \tag{8}$$

In the above, $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$, m/M is the electron to nuclear mass ratio, Z is the nuclear charge, H is the external magnetic field with its Z component being H_Z, μ_B is the Bohr magneton, $C_k^q=\sqrt{4\pi/(2k+1)}\;Y_k^q(\mathbf{r})$, $\mathbf{L}$ is the total orbital angular momentum operator, $\mathbf{S}=\Sigma_i\mathbf{s}_i$ is the total spin angular momentum operator, and g_L and g_S [14] are

$$g_L=1-m/M, \tag{9}$$

$$g_S=2[1+\alpha/2\pi-0.328\,478\,965(\alpha/\pi)^2$$

$$+1.181\,241\,456(\alpha/\pi)^3+\cdots]. \tag{10}$$

TABLE I. Convergence of the reduced matrix elements F_i for the $2\,^2P$ state of lithium. N is the number of terms in the wave function. Units are atomic units.

N	F_1	F_2	F_3	F_4	F_5	F_6
56	−0.196 475	−0.071 3144	−1.018 278 75	−0.021 907 26	−0.579 9228	0.564 388 11
139	−0.203 462	−0.073 8071	−1.019 044 63	−0.021 849 39	−0.580 5921	0.564 559 24
307	−0.204 664	−0.074 1102	−1.019 145 49	−0.021 845 18	−0.580 6623	0.564 593 34
623	−0.205 097	−0.074 1936	−1.019 153 92	−0.021 845 78	−0.580 6622	0.564 597 82
1175	−0.205 364	−0.074 2363	−1.019 156 40	−0.021 845 96	−0.580 6996	0.564 604 51
1846	−0.205 426	−0.074 2452	−1.019 156 34	−0.021 846 14	−0.580 6911	0.564 603 03
2882	−0.205 489	−0.074 2532	−1.019 156 09	−0.021 846 02	−0.580 7003	0.564 604 67
3463	−0.205 493	−0.074 2537	−1.019 156 18	−0.021 846 06	−0.580 7004	0.564 604 70
∞	−0.205 493(4)	−0.074 2537(5)	−1.019 156 18(9)	−0.021 846 06(4)	−0.580 7004(1)	0.564 604 70(3)

N	F_7	F_8	F_9	F_{10}	F_{11}
56	1.128 355 83	−0.364 2220	−0.528 5319	68.564 451	−41.972 447
139	1.128 638 38	−0.364 2944	−0.528 7621	68.472 014	−41.913 877
307	1.128 706 33	−0.364 2945	−0.528 8092	68.460 940	−41.906 744
623	1.128 714 73	−0.364 2948	−0.528 8197	68.459 350	−41.905 730
1175	1.128 718 46	−0.364 2939	−0.528 8251	68.459 016	−41.905 510
1846	1.128 717 27	−0.364 2933	−0.528 8265	68.458 935	−41.905 457
2882	1.128 718 06	−0.364 2932	−0.528 8267	68.458 922	−41.905 448
3463	1.128 718 09	−0.364 2931	−0.528 8268	68.458 919	−41.905 446
∞	1.128 718 09(3)	−0.364 2931(1)	−0.528 8268(1)	68.458 919(3)	−41.905 446(2)

TABLE II. Reduced matrix elements F_i for the $2\,^2P$ states of lithiumlike ions. Units are atomic units.

Term	Li	Be^+	B^{2+}	C^{3+}	N^{4+}
F_1	−0.205 493(4)	−0.526 20(1)	−0.734 673(3)	−0.869 7211(2)	−0.962 6148(2)
F_2	−0.074 2537(5)	−0.322 199(2)	−0.617 6277(8)	−0.924 5113(2)	−1.234 8035(2)
F_3	−1.019 156 18(9)	−4.095 720 2(1)	−9.012 1014(2)	−15.696 8520(2)	−24.129 3635(2)
F_4	−0.021 846 06(4)	−0.060 596 0(2)	−0.101 7831(2)	−0.143 9617(3)	−0.186 6840(3)
F_5	−0.580 7004(1)	−2.346 40(1)	−5.228485(5)	−9.194 131(4)	−14.231 577(3)
F_6	0.564 604 70(3)	1.127 791(1)	1.676 3909(6)	2.217 9593(3)	2.755 8525(2)
F_7	1.128 718 09(3)	2.229 965 4(5)	3.283 0886(3)	4.313 7863(1)	5.333 0681(1)
F_8	−0.364 2931(1)	−0.733 728 6(3)	−1.089 8777(1)	−1.438 5481(3)	−1.783 0648(2)
F_9	−0.528 8268(1)	−0.994 984 270(5)	−1.433 3686(1)	−1.860 82895(4)	−2.283 0654(1)
F_{10}	68.458 919(3)	17.534 032 8(8)	8.072 59935(8)	4.672 72614(5)	3.057 306 69(2)
F_{11}	−41.905 446(2)	−10.362 610(1)	−4.660 5788(1)	−2.655 34424(6)	−1.717 895 16(4)

Term	O^{5+}	F^{6+}	Ne^{7+}	Na^{8+}	Mg^{9+}
F_1	−1.029 9923(1)	−1.080 951(2)	−1.120 7844(1)	−1.152 7495(4)	−1.178 9552(4)
F_2	−1.546 2220(1)	−1.858 0015(4)	−2.169 8596(2)	−2.481 6881(1)	−2.793 4478(1)
F_3	−34.301 9763(3)	−46.211 26859(4)	−59.855 5010(2)	−75.233 7023(2)	−92.345 2895(2)
F_4	−0.229 7388(3)	−0.273 0117(3)	−0.316 4352(3)	−0.359 9670(3)	−0.403 5793(3)
F_5	−20.335 859(4)	−27.504558(8)	−35.736365(5)	−45.03051(1)	−55.386 526(5)
F_6	3.291 6097(3)	3.826 0207(4)	4.359530(1)	4.892 4063(2)	5.424 8213(1)
F_7	6.345 85706(4)	7.354 6250(1)	8.360 737013(3)	9.365 0058(1)	10.367 9443(2)
F_8	−2.125 0906(3)	−2.465 5165(3)	−2.804 8572(3)	−3.143 4293(3)	−3.481 4374(3)
F_9	−2.702 4255(1)	−3.120 0390(1)	−3.536 514 21(2)	−3.952 2069(1)	−4.367 3390(2)
F_{10}	2.159 926 20(1)	1.608 67301(1)	1.245 31354(1)	0.992 94694(1)	0.810 439 640(3)
F_{11}	−1.203 528 42(2)	−0.890 59044(2)	−0.685 90043(1)	−0.544 62627(1)	−0.442 990 650(6)

TABLE III. Reduced matrix elements F_i for the $3\,^2P$ states of lithiumlike ions. Units are atomic units.

Term	Li	Be^+	B^{2+}	C^{3+}	N^{4+}
F_1	−0.060 499(5)	−0.1387(2)	−0.1806(2)	−0.2042(1)	−0.218 98(8)
F_2	−0.024 145(4)	−0.093 18(3)	−0.167 65(3)	−0.241 26(3)	−0.313 68(3)
F_3	−0.432 6520(3)	−1.724 7491(1)	−3.810 3377(2)	−6.672 685 67(2)	−10.307 6316(4)
F_4	−0.005 5274(2)	−0.015 5559(2)	−0.027 6038(6)	−0.040 8986(6)	−0.054 948(1)
F_5	−0.251 558(1)	−1.012 09(1)	−2.259 85(2)	−3.985 29(2)	−6.185 12(3)
F_6	0.246 4317(2)	0.491 653(1)	0.732 534(1)	0.971 426(2)	1.209 287(2)
F_7	0.492 5074(1)	0.974 7267(2)	1.443 4929(2)	1.906 624(1)	2.367 037(1)
F_8	−0.158 100 798(1)	−0.316 6572(1)	−0.471 0692(4)	−0.623 4161(2)	−0.774 680 9(2)
F_9	−0.240 2827(2)	−0.465 1756(5)	−0.682 488(1)	−0.896 5657(4)	−1.108 9898(4)
F_{10}	415.1954(3)	103.855 510(7)	46.719 393(6)	26.570 466(4)	17.155 89(1)
F_{11}	−261.2073(2)	−64.962 85(1)	−29.106 72(1)	−16.507 143(2)	−10.636 277(1)

Term	O^{5+}	F^{6+}	Ne^{7+}	Na^{8+}	Mg^{9+}
F_1	−0.228 88(6)	−0.235 90(4)	−0.241 12(4)	−0.245 13(4)	−0.248 31(3)
F_2	−0.385 18(2)	−0.456 00(1)	−0.526 34(2)	−0.596 31(2)	−0.665 99(2)
F_3	−14.713 7466(2)	−19.890 4223(5)	−25.837 3607(4)	−32.554 3995(3)	−40.0414 436(5)
F_4	−0.069 4768(6)	−0.084 3254(4)	−0.099 3976(5)	−0.114 631 6(5)	−0.129 9866(5)
F_5	−8.858 00(3)	−12.003 28(4)	−15.6205(1)	−19.709 75(5)	−24.270 62(5)
F_6	1.446 545(2)	1.683 423(2)	1.920 044(2)	2.156 484(2)	2.392 791(3)
F_7	2.825 950(1)	3.283 9520(5)	3.741 360(1)	4.198 361(1)	4.655 0702(6)
F_8	−0.925 3190(5)	−1.075 5642(6)	−1.225 5471(6)	−1.375 346(1)	−1.525 012(1)
F_9	−1.320 4568(7)	−1.531 319(1)	−1.741 776(1)	−1.951 947(1)	−2.161 910(1)
F_{10}	11.997 620(1)	8.864 3485(1)	6.818 0269(1)	5.407 6478(2)	4.394 253 89(3)
F_{11}	−7.426 5859(2)	−5.480 3161(1)	−4.211 0143(1)	−3.337 2017(2)	−2.709 963 01(5)

TABLE IV. Comparison of $\langle H_i \rangle$ for the $2\,^2P_J$ and $3\,^2P_J$ states of lithium, where $\langle H_i \rangle = \langle LSJJ|H_i|LSJJ \rangle$. The first entry is the present calculation and the second entry is the value of Guan and Wang [5]. Units are $10^{-6}\mu_B H(-J)$ a.u.

Term	$2\,^2P_{1/2}$	$2\,^2P_{3/2}$	$3\,^2P_{1/2}$	$3\,^2P_{3/2}$
$\langle H_1 \rangle$	5.585 450(1)	10.081 3666(9)	2.328 96(1)	4.321 90(1)
	5.5826	10.0800	2.3291	4.3206
$\langle H_2 \rangle$	14.363 903(3)	−5.688 3598(3)	6.245 528(2)	−2.480 400(2)
	14.363	−5.6800	6.2459	−2.4802
$\langle H_3 \rangle$	−8.860 931(1)	3.719 5061(2)	−3.969 383(3)	1.633 2762(3)
	−8.8651	3.7195	−7.6890	2.0051
$\langle H_4 \rangle$	−0.537 085(5)	−0.268 542(3)	−0.190 80(4)	−0.095 40(2)
	0.099 81	0.049 90	0.120 60	0.060 30
$\langle H_5 \rangle$	−6.1858(1)	−3.092 91(5)	−1.8211(1)	−0.910 58(6)
	61.4888	30.7444	1.6195	0.8097

The application of angular momentum algebra yields the expression for the matrix element of the Zeeman Hamiltonian between J' and J:

$$\begin{aligned}\langle LSJ'M_J|H_{\text{Zeeman}}|LSJM_J\rangle=(\mu_B H)(-1)^{1-M_J}(J,J')^{1/2}\begin{pmatrix} J' & 1 & J \\ -M_J & 0 & M_J\end{pmatrix}\sqrt{6}\Bigg[\begin{Bmatrix} L & J' & S \\ J & L & 1\end{Bmatrix}(-1)^{J+J'+L+S}g'_L \\ +\begin{Bmatrix} J & J' & 1 \\ S & S & L\end{Bmatrix}(-1)^{L+S}g'_S+(-1)^{J'}\begin{Bmatrix} L & L & 2 \\ S & S & 1 \\ J' & J & 1\end{Bmatrix}g_X\Bigg] \\ +\frac{2}{3}(\mu_B H)^2(-1)^{J+J'-M_J}(J,J')^{1/2}\Bigg[\begin{pmatrix} J' & 0 & J \\ -M_J & 0 & M_J\end{pmatrix}\begin{Bmatrix} L & J' & S \\ J & L & 0\end{Bmatrix}(-1)^{L+S}g_{Q1} \\ -\begin{pmatrix} J' & 2 & J \\ -M_J & 0 & M_J\end{pmatrix}\begin{Bmatrix} L & J' & S \\ J & L & 2\end{Bmatrix}(-1)^{L+S}g_{Q2}\Bigg],\end{aligned} \tag{11}$$

where $(\alpha,\beta,\dots)=(2\alpha+1)(2\beta+1)\dots$. 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

$$\begin{aligned}g'_L=&\sqrt{\frac{(2L+1)L(L+1)}{6}}\ g_L-\frac{1}{\sqrt{6(2S+1)}}\frac{m}{M}F_1 \\ &+\frac{\alpha^2}{2\sqrt{6(2S+1)}}(-F_2+F_3+F_4),\end{aligned} \tag{12}$$

$$\begin{aligned}g'_S=&\sqrt{\frac{(2S+1)S(S+1)}{6}}g_S(-1)^{2J'} \\ &+\frac{\alpha^2}{\sqrt{6(2L+1)}}(-1)^{2J'}\left(F_5+\frac{Z}{3}F_6-\frac{1}{3}F_7\right),\end{aligned} \tag{13}$$

$$g_X=\frac{\sqrt{5}}{6}\alpha^2\left(-ZF_8+\frac{\sqrt{6}}{2}F_9\right), \tag{14}$$

$$g_{Q1}=\frac{1}{2\sqrt{2S+1}}F_{10}, \tag{15}$$

$$g_{Q2}=\frac{1}{2\sqrt{2S+1}}F_{11}. \tag{16}$$

The reduced matrix elements F_i are defined by

$$F_1=\sum_{j\neq k}\langle\Psi||-i\mathbf{r}_j\times\boldsymbol{\nabla}_k||\Psi\rangle\langle S||1||S\rangle, \tag{17}$$

$$F_2=\sum_{k>j}\langle\Psi||-i\frac{1}{r_{jk}}(\mathbf{r}_j\times\boldsymbol{\nabla}_k+\mathbf{r}_k\times\boldsymbol{\nabla}_j)||\Psi\rangle\langle S||1||S\rangle, \tag{18}$$

$$F_3=\sum_j\langle\Psi||\nabla_j^2(-i\mathbf{r}_j\times\boldsymbol{\nabla}_j)||\Psi\rangle\langle S||1||S\rangle, \tag{19}$$

$$F_4=\sum_{k>j}\langle\Psi||-i\frac{1}{r_{jk}^3}(\mathbf{r}_j\times\mathbf{r}_k)[\mathbf{r}_{jk}\cdot(\boldsymbol{\nabla}_j+\boldsymbol{\nabla}_k)]||\Psi\rangle\langle S||1||S\rangle, \tag{20}$$

$$F_5=\sum_j\langle\Psi||\nabla_j^2||\Psi\rangle\langle S||\mathbf{s}_j||S\rangle, \tag{21}$$

$$F_6=\sum_j\langle\Psi||\frac{1}{r_j}||\Psi\rangle\langle S||\mathbf{s}_j||S\rangle, \tag{22}$$

$$F_7=\sum_{j\neq k}\langle\Psi||\frac{(\mathbf{r}_j\cdot\mathbf{r}_{jk})}{r_{jk}^3}||\Psi\rangle\langle S||(\mathbf{s}_j+2\mathbf{s}_k)||S\rangle, \tag{23}$$

$$F_8=\sum_j\langle\Psi||\frac{1}{r_j}C_2(\mathbf{r}_j)||\Psi\rangle\langle S||\mathbf{s}_j||S\rangle, \tag{24}$$

$$F_9=\sum_{j\neq k}\langle\Psi||\frac{1}{r_{jk}^3}(\mathbf{r}_j\otimes\mathbf{r}_{jk})^{(2)}||\Psi\rangle\langle S||(\mathbf{s}_j+2\mathbf{s}_k)||S\rangle, \tag{25}$$

$$F_{10}=\sum_j\langle\Psi||r_j^2||\Psi\rangle\langle S||1||S\rangle, \tag{26}$$

$$F_{11}=\sum_j\langle\Psi||r_j^2C_2(\mathbf{r}_j)||\Psi\rangle\langle S||1||S\rangle. \tag{27}$$

For the operator H_3, a recoupling procedure was applied in order to separate the orbital and spin parts (see [15], p. 85). It is easy to show that the formulation for a two-electron system [12] is contained here as a special case.

III. CALCULATIONS AND RESULTS

We consider a lithiumlike ion for the case of infinite nuclear mass. The wave functions for lithiumlike ions were constructed variationally in multiple basis sets in Hylleraas coordinates containing terms of the form

$$r_1^{j_1} r_2^{j_2} r_3^{j_3} r_{12}^{j_{12}} r_{23}^{j_{23}} r_{31}^{j_{31}} e^{-\alpha r_1 - \beta r_2 - \gamma r_3} \mathcal{Y}^{LM}_{(\ell_1 \ell_2)\ell_{12},\ell_3}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\chi_1, \tag{28}$$

where $\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}$ is a vector-coupled product of spherical harmonics for the three electrons to form a state of total angular momentum L, and χ_1 is a spin function with spin angular momentum 1/2. As described previously [16], all terms from Eq. (28) are nominally included such that

$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leq \Omega, \tag{29}$$

and the convergence of the eigenvalues is studied as Ω is progressively increased. The computational details of all necessary integrals, including singular integrals, can be found in [17]. Note that for S states the only nonzero terms are F_5, F_6, F_7, and F_{10} due to the triangular rule of angular momen-

TABLE V. Contributions to the g_J factors for lithium and lithiumlike ions in the $2\,^2P_J$ and $3\,^2P_J$ states. α^0 indicates the terms involving g_L, g_S, and F_1, and α^2 indicates the relativistic correction of order α^2.

Term	$2\,^2P_{1/2}$	$2\,^2P_{3/2}$	$3\,^2P_{1/2}$	$3\,^2P_{3/2}$
		^{7}Li		
α^0	−0.665 795 4734(1)	−1.334 057 388 96(5)	−0.665 791 1088(1)	−1.334 055 206 63(6)
α^2	0.000 010 551 336(6)	0.000 007 843 970(3)	0.000 004 41430(4)	0.000 003 379 38(2)
g_J	−0.665 784 9221(1)	−1.334 049 544 99(5)	−0.665 786 6945(1)	−1.334 051 827 25(6)
		^{9}Be$^+$		
α^0	−0.665 824 7157(3)	−1.334 072 0101(1)	−0.665 815 635(3)	−1.334 067 469(2)
α^2	0.000 041 160 15(6)	0.000 031 403 71(6)	0.000 017 3247(2)	0.000 013 527 6(1)
g_J	−0.665 783 5556(3)	−1.334 040 6063(1)	−0.665 798 310(3)	−1.334 053 942(2)
		^{11}B^{2+}		
α^0	−0.665 841 204 17(5)	−1.334 080 254 31(3)	−0.665 830 575(2)	−1.334 074 939(1)
α^2	0.000 090 124 30(4)	0.000 069 805 96(4)	0.000 038 2961(3)	0.000 030 1866(2)
g_J	−0.665 751 079 87(7)	−1.334 010 448 35(5)	−0.665 792 278(2)	−1.334 044 753(1)
		^{12}C^{3+}		
α^0	−0.665 847 902 699(4)	−1.334 083 603 576(2)	−0.665 836 190(2)	−1.334 077 7474(9)
α^2	0.000 157 047 11(3)	0.000 122 677 07(3)	0.000 067 2284(3)	0.000 053 2426(2)
g_J	−0.665 690 855 58(3)	−1.333 960 926 50(3)	−0.665 768 962(2)	−1.334 024 5048(9)
		^{14}N^{4+}		
α^0	−0.665 855 835 608(2)	−1.334 087 570 030(1)	−0.665 844 619(1)	−1.334 081 9620(6)
α^2	0.000 241 815 45(3)	0.000 189 881 43(3)	0.000 104 0873(4)	0.000 082 6530(3)
g_J	−0.665 614 020 14(3)	−1.333 897 688 59(3)	−0.665 740 532(1)	−1.333 999 3089(7)
		^{16}O^{5+}		
α^0	−0.665 861 423 747(1)	−1.334 090 364 1001(5)	−0.665 850 8454(8)	−1.334 085 0749(4)
α^2	0.000 344 385 54(4)	0.000 271 360 77(4)	0.000 148 8575(3)	0.000 118 3993(3)
g_J	−0.665 517 038 20(4)	−1.333 819 003 32(4)	−0.665 701 9878(9)	−1.333 966 6755(5)
		^{19}F^{6+}		
α^0	−0.665 867 071 94(1)	−1.334 093 188 198(7)	−0.665 857 6776(5)	−1.334 088 4910(2)
α^2	0.000 464 736 87(7)	0.000 367 086 33(6)	0.000 201 5312(4)	0.000160 4723(4)
g_J	−0.665 402 335 07(7)	−1.333 726 101 85(6)	−0.665 656 1464(6)	−1.333 928 0187(4)
		^{20}Ne^{7+}		
α^0	−0.665 868 809 6388(6)	−1.334 094 057 0457(3)	−0.665 859 5166(4)	−1.334 089 4105(2)
α^2	0.000 602 858 61(5)	0.000 477 042 39(4)	0.000 262 1037(4)	0.000 208 8666(4)
g_J	−0.665 265 951 02(5)	−1.333 617 014 65(4)	−0.665 597 4129(6)	−1.333 880 5438(4)
		^{23}Na^{8+}		
α^0	−0.665 872 331 097(4)	−1.334 095 817 775(2)	−0.665 863 9929(3)	−1.334 091 6487(1)
α^2	0.000 758 744 46(6)	0.000 601 219 64(5)	0.000 330 5722(5)	0.000 263 5793(5)
g_J	−0.665 113 586 63(6)	−1.333 494 598 13(5)	−0.665 533 4207(6)	−1.333 828 0694(5)
		^{24}Mg^{9+}		
α^0	−0.665 873 442 737(4)	−1.334 096 373 594(2)	−0.665 865 2477(3)	−1.334 092 2760(1)
α^2	0.000 932 390 52(5)	0.000 739 612 23(4)	0.000 406 9350(5)	0.000 324 6083(5)
g_J	−0.664 941 052 21(5)	−1.333 356 761 35(4)	−0.665 458 3126(6)	−1.333 767 6677(5)

tum. Table I is the results of the convergence studies of the reduced matrix elements F_i for the $2\,^2P$ state of lithium, as the size of the basis set is enlarged up to 3463. The results corresponding to $N=3463$ are taken as the values of extrapolation to $N\rightarrow\infty$, with the differences of the last two calculations being the uncertainties. Tables II and III list the reduced matrix elements F_i for the $2\,^2P$ and $3\,^2P$ states of lithiumlike ions, respectively, with Z up to 12. The consistency of our values can be checked as follows. Since each F_i is a homogeneous function in $\mathbf{r}$ space, it can be expanded into a series in powers of Z^{-1} according to the method of large-Z expansion [16]. Consider F_4 for example. A fit to our numerical results in the range $Z=3$ to 11 for the state of $2\,^2P$ yields

$$F_4=-0.044\,020(26)Z+0.129\,472(81)-0.0617(16)Z^{-1}+0.0609(37)Z^{-2}-0.147(26)Z^{-3}. \tag{30}$$

This equation predicts $F_4=-0.403\,57(35)$ for the case of $Z=12$, in comparison with the directly calculated result of $-0.403\,5793(3)$. Table IV is the comparison of our matrix elements of H_i with the calculations of Guan and Wang [5] for the $2\,^2P_J$ and $3\,^2P_J$ states of lithium. Our results for H_1 and H_2 agree with but are much more accurate than the values of Guan and Wang. For H_3, a similar agreement exists only for the $2\,^2P_{1/2}$ and $2\,^2P_{3/2}$ states; there are large discrepancies, however, for the $3\,^2P_{1/2}$ and $3\,^2P_{3/2}$ states. For H_4 and H_5, their calculations completely disagree with ours. For the operator H_4, their expression [Eq. (6) of [5]] seems to be in error [10]:

$$H_4^{(\mathrm{GW})}=-\alpha^2\mu_B\mathbf{H}\cdot\sum_{i\neq j}^{3}[(\mathbf{r}_i\times\mathbf{p}_i)/r_{ij}+(\mathbf{r}_i\times\mathbf{r}_j)(\mathbf{r}_{ij}\cdot\mathbf{p}_j)/r_{ij}^3]. \tag{31}$$

First, an overall factor of 1/2 is missing from the above expression. Secondly, $\mathbf{r}_i\times\mathbf{p}_i$ should be replaced by $\mathbf{r}_i\times\mathbf{p}_j$. Thirdly, the definition of $\mathbf{r}_{ij}$ is not given in their paper. If their definition is the same as ours, $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$, then the second term of their expression should have a sign change [18]. No obvious explanation can be found for the disagreement for H_5. Table V summaries the contributions to the g_J factors for lithium and lithiumlike ions. The diagonal g_J factor can be defined by

$$g_J=-\lim_{H\rightarrow 0}\frac{\langle LSJJ|H_{\mathrm{Zeeman}}|LSJJ\rangle}{\mu_B HJ}. \tag{32}$$

Thus the contribution from the quadratic term H_6 can be ignored. To the best of our knowledge, the only measurements for the $2\,^2P_{1/2}$ and $2\,^2P_{3/2}$ states of lithium are due to Ritter [19] using the optical-radio-frequency double-resonance method. His results are $-0.6668(20)$ and $-1.335(10)$, respectively (see also the review article by Arimondo *et al.* [20]). Although our calculations agree with the measurements, the uncertainties in the experimental values are too large to provide a meaningful test for the relativistic effects of order α^2. It should be mentioned here that all the uncertainties assigned in Table V are purely computational and have nothing to do with the uncalculated higher-order terms.

In summary, we have performed high-precision calculations of the Zeeman g_J factors for lithium and lithiumlike ions in the $2\,^2P_J$ and $3\,^2P_J$ states using variational wave functions in fully correlated Hylleraas coordinates, including the lowest-order relativistic corrections. The next higher-order effects not included in the present calculations are relativistic recoil corrections of order $\alpha^2 m/M$ and radiative corrections of order α^3. No theoretical analysis has been carried out on these effects to our knowledge for a three-electron system in an external magnetic field. We hope that our work will stimulate further research activities in both theory and experiment.

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