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Calculation of the g_J Factor for the $2\,^3S_1$ State of Helium

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The g_J factor for the excited $2\,^3S_1$ state of helium has been calculated from a generalized Breit equation which includes radiative corrections. The result is $g_J\,(\mathrm{He}, 2\,^3S_1) = g_e(1-40.91640\times10^{-6}) = -2.002237379$. This result is in good agreement with the previous theoretical value calculated by Perl and Hughes to order α^2. Higher-order corrections (α^3 and $\alpha^2 m/M$) contribute -0.151 ppm. Combining this result with the calculated value for the atomic hydrogen g_J factor gives the ratio $g_J(\mathrm{He}, 2\,^3S_1)/g_J(\mathrm{H}, 1\,^2S_{1/2}) = 1-23.212\times10^{-6}$ with an estimated uncertainty of 3×10^{-9}. This value is in agreement with the old experimental and theoretical values of Hughes *et al.*, and improves upon the accuracy of the latter, but disagrees with a recent experimental value obtained by Leduc, Laloë, and Brossel.

I. INTRODUCTION

In recent years there has been a remarkable increase in the precision of measurements of atomic magnetic moments. In some cases, atomic g-factor ratios have been measured to 0.1 ppm or better.[1,2] In order to understand these results from the point of view of theory, it is necessary to consider not only the dominant $\alpha^2 \sim 50$ ppm relativistic bound-state contributions to the g factors, but also bound-state radiative corrections, of order $\alpha^3 \sim 0.1$ ppm, and nuclear mass corrections, of order $\alpha^2 m/M \sim 0.01\, M_p/M$ ppm. (α is the fine-structure constant, and m, M, and M_p the electron, nuclear, and proton masses, respectively). The consideration of all these contributions in the theory[3] has led to excellent agreement between theory and experiment for hydrogenic atoms; for the hydrogen/deuterium g factor ratio, for example, theory and experiment[2b] agree to one part in 10^{11}.

The theory, based on a generalized Breit equation which includes radiative corrections, may be extended to include many-electron atoms.[4] We report here a calculation of the g factor of the $2\,^3S_1$ state of the helium atom. This calculation is of interest because there is a rather large disagreement (2 ppm) between a recent precise experimental determination[5] of the ratio $g_J(\mathrm{He}, 2\,^3S_1)/g_J(\mathrm{H}, 1^2S_{\frac12})$ and a theoretical calculation[6] of this ratio to order α^2. In Sec. II we present the calculation of $g_J(\mathrm{He}, 2^3S_1)$ and the above ratio to orders α^3 and $\alpha^2 m/M$, and in Sec. III we summarize the results and compare them with the earlier experimental and theoretical work.

II. CALCULATIONS

In performing the calculations we use first-order perturbation theory with the Hamiltonian given in Eq. (21) of Ref. 4, and with the unperturbed wave function taken to be the 715-term function obtained by Pekeris[7] for the $2\,^3S$ state of helium. The g factor is defined[8] by

$$g_J(2\,^3S_1) = -\langle 2\,^3S_1 | \mathcal{H}' | 2\,^3S_1\rangle / \mu_B H, \qquad (1)$$

where the matrix element is evaluated in the "stretched" state $J = M_J = 1$, $\mathcal{H}'$ is the magnetic-field-dependent part of $\mathcal{H}_3 + \mathcal{H}_4 + \mathcal{H}_5$ given in Eq. (21) of Ref. 4, μ_B is the Bohr magneton, and H is the external magnetic field.

We consider the contributions of each term in the Hamiltonian separately. For a heliumlike atom, the magnetic-field-dependent part of the spin-orbit coupling term $\mathcal{H}_3$ is

$$\mathcal{H}_3' = -(Ze^2/m)\,\mu_B(g_e+1)\,(\vec{S}_1\cdot\vec{r}_1\times\vec{A}_1/r_1^3 + \vec{S}_2\cdot\vec{r}_2\times\vec{A}_2/r_2^3) + (e^2/m)\,\mu_B(g_e+1)\,(\vec{S}_1\cdot\vec{r}_{12}\times\vec{A}_1/r_{12}^3 + \vec{S}_2\cdot\vec{r}_{21}\times\vec{A}_2/r_{12}^3), \qquad (2)$$

where $g_e \cong -2$ is the free-electron g factor, $\vec{A}_1 = \vec{H}\times\vec{r}_1/2$, etc., and the other symbols have their usual meanings. All electron coordinates with only one subscript (e.g., $\vec{r}_1$) are understood to be measured with respect to the nucleus. The matrix element of this operator can be evaluated in a manner similar to that of Perl and Hughes.[6] Then, using Eq. (1), we find the contribution of $\mathcal{H}_3'$ to the g factor

$$g_{J3} = -\frac{g_e+1}{6m}\langle 2\,^3S| -\frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}}|2\,^3S\rangle$$
$$= -\tfrac{1}{3}(g_e+1)\frac{E(2\,^3S)}{m}, \quad (3)$$

where we have used the virial theorem $\langle V\rangle = 2E$, where E is the total nonrelativistic electronic energy.

We next evaluate the contribution from the spin-other-orbit coupling term

$$\mathcal{H}_4' = \frac{Ze^2}{M}\mu_B g_e\left(\vec{S}_1\cdot\vec{r}_1\times\frac{\vec{A}_1}{r_1^3} + \vec{S}_2\cdot\vec{r}_2\times\frac{\vec{A}_2}{r_2^3} + \vec{S}_1\cdot\vec{r}_1\times\frac{\vec{A}_2}{r_1^3} + \vec{S}_2\cdot\vec{r}_2\times\frac{\vec{A}_1}{r_2^3}\right) - \frac{e^2}{m}\mu_B g_e\left(\vec{S}_1\cdot\vec{r}_{12}\times\frac{\vec{A}_2}{r_{12}^3} - \vec{S}_2\cdot\vec{r}_{12}\times\frac{\vec{A}_1}{r_{12}^3}\right). \quad (4)$$

Again following the method of Perl and Hughes,[6] and using Eq. (1), we obtain

$$g_{J4} = -\frac{g_e}{6m}\langle 2\,^3S|\frac{e^2}{r_{12}} + \frac{m}{M}\left(\frac{Ze^2}{r_1} + \frac{Ze^2}{r_2} + \frac{Ze^2\,\vec{r}_1\cdot\vec{r}_2}{r_1^3} + \frac{Ze^2\,\vec{r}_1\cdot\vec{r}_2}{r_2^3}\right)|2\,^3S\rangle\,. \quad (5)$$

Finally, we consider $\mathcal{H}_5$, which describes the direct interaction of the electron spins with the external magnetic field and relativistic mass corrections to this interaction:

$$\mathcal{H}_5' = -\mu_B g_e\vec{H}\cdot[\vec{S}_1(1-p_1^2/2m^2) + \vec{S}_2(1-p_2^2/2m^2)] - (1/2m^2)\mu_B(g_e+2)(\vec{H}\cdot\vec{S}_1p_1^2 - \vec{H}\cdot\vec{p}_1\vec{p}_1\cdot\vec{S}_1 + \vec{H}\cdot\vec{S}_2p_2^2 - \vec{H}\cdot\vec{p}_2\vec{p}_2\cdot\vec{S}_2)\cdot \quad (6)$$

The corresponding contribution to the g factor is

$$g_{J5} = g_e[1-(m_r/2m^2)\langle 2\,^3S|p_1^2/2m_r + p_2^2/2m_r|2\,^3S\rangle] + (m_r/3m^2)(g_e+2)\langle 2\,^3S|p_1^2/2m_r + p_2^2/2m_r|2\,^3S\rangle\cdot \quad (7)$$

Again using the virial theorem $\langle T\rangle = -E$, we obtain

$$g_{J5} = g_e\left(1+\frac{m_r}{2m^2}E(2\,^3S)\right) - \tfrac{1}{3}(g_e+2)\frac{m_r}{m^2}E(2\,^3S). \quad (8)$$

Summing $g_J(2\,^3S_1) = g_{J3} + g_{J4} + g_{J5}$, factoring out g_e, and expanding $g_e = -2(1+\alpha/2\pi\ldots)$ to order α, we obtain, correct to order α^3,

$$g_J(2\,^3S_1) = g_e\left[1 + \frac{1}{2}\left(\frac{m_r}{m} - \frac{1}{3}\right)\frac{E(2\,^3S)}{m} - \frac{\alpha}{6\pi}\left(\frac{m_r}{m} + \frac{1}{2}\right)\frac{E(2\,^3S)}{m} - \frac{1}{6}\frac{\langle 2\,^3S|V'|2\,^3S\rangle}{m}\right] \quad (9)$$

where

$$V' = \frac{e^2}{r_{12}} + \frac{m}{M}\left(\frac{Ze^2}{r_1} + \frac{Ze^2}{r_2}\right) + \frac{m}{M}Ze^2\left(\frac{\vec{r}_1\cdot\vec{r}_2}{r_1^3} + \frac{\vec{r}_1\cdot\vec{r}_2}{r_2^3}\right). \quad (10)$$

We now exhibit all the nuclear mass corrections explicitly by using $m_r = mM/(M+m) \cong m(1-m/M)$ to write

$$E(2\,^3S) = E_\infty(2\,^3S)(1-m/M),$$
$$\langle 2\,^3S|1/r|2\,^3S\rangle = \langle 2\,^3S|1/r|2\,^3S\rangle_\infty(1-m/M), \quad (11)$$

where the subscript ∞ denotes quantities calculated assuming infinite nuclear mass. Substituting these expressions into Eq. (9), we obtain, correct to orders α^3 and $\alpha^2 m/M$,

$$g_J(2\,^3S_1) = g_e\left[1 + \frac{1}{3}\frac{E_\infty}{m} - \frac{1}{6m}\left\langle\frac{e^2}{r_{12}}\right\rangle_\infty - \frac{\alpha}{4\pi}\frac{E_\infty}{m} + \frac{1}{6M}\left(-5E_\infty + \left\langle\frac{e^2}{r_{12}} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2}\right\rangle_\infty\right) - \frac{Z\alpha}{6M}\left\langle\frac{\vec{r}_1\cdot\vec{r}_2}{r_1^3} + \frac{\vec{r}_1\cdot\vec{r}_2}{r_2^3}\right\rangle_\infty\right], \quad (12)$$

where all energies and expectation values refer to the $2\,^3S$ state. The second line of Eq. (12) can be expressed in terms of E_∞ by applying the virial theorem $\langle V\rangle_\infty = 2E_\infty$. The third line of Eq. (12), which is formally of order $\alpha^2 m/M$, but which we estimate to be less than $g_e\times 0.001$ ppm, is negligible for our purposes.[9] Our final expression is then

$$g_J(2\,^3S) = g_e\left(1 + \frac{1}{3}\frac{E_\infty}{m} - \frac{1}{6m}\left\langle\frac{e^2}{r_{12}}\right\rangle_\infty - \frac{\alpha}{4\pi}\frac{E_\infty}{m} - \frac{1}{2}\frac{m}{M}\frac{E_\infty}{m}\right). \quad (13)$$

Using the results of Pekeris[7] for the $2\,^3S$ state of helium: $E_\infty = -2.175\,229\,378\,24\alpha^2 m$ and $\langle 1/r_{12}\rangle_\infty = 0.268\,197\,855\,3\alpha m$, and taking $\alpha^{-1} = 137.036\,02$, we obtain[9a]

$$g_J(\text{He}, 2\,^3S_1) = g_e(1 - 40.991\,61\times 10^{-6} + 0.067\,27\times 10^{-6} + 0.007\,94\times 10^{-6}), \quad (14)$$

where the second term in parentheses on the right-hand side of Eq. (14) is the α^2 contribution from Eq. (13), the third term is the α^3 contribution, and the fourth term is the $\alpha^2 m/M$ contribution. The estimated uncertainty of the quantity in parentheses is 3×10^{-9}, and arises due to the neglect of α^4 corrections and the third line of Eq. (12). Using the recent theoretical value[10] $g_e = -2[1+\alpha/2\pi - 0.328\,48$

$(\alpha/\pi)^2+1.29\,(\alpha/\pi)^3]$, we obtain the numerial result

$$\begin{aligned} g_J(\mathrm{He},\,2\,^3S_1) &= -2.002\,237\,228 - 0.000\,000\,135 \\ &\quad - 0.000\,000\,016, \\ &= -2.002\,237\,379, \end{aligned} \qquad (15)$$

where the α^3 contribution is seen to be -0.135 ppm. The α^2 contribution is in excellent agreement with the previous theoretical value.[6]

To make further comparison we calculate the ratio

$$\frac{g_J(\mathrm{He},\,2\,^3S_1)}{g_J(\mathrm{H},\,1^2S_{\frac{1}{2}})} = \frac{g_e(1-40.9164\times10^{-6})}{g_e\,(1-17.7051\times10^{-6})} = 1-23.212\times10^{-6}, \qquad (16)$$

where we have used the hydrogen g factor calculated in Ref. 3. Equation (16) is in agreement with the previous theoretical value[6] for this g-factor ratio, and improves upon the accuracy of the latter.

III. SUMMARY AND CONCLUSIONS

Our final results are given in Eqs. (13), (15), and (16). The estimated uncertainty in $g_J\,(\mathrm{He},\,2\,^3S_1)$ is 7×10^{-9}, due principally to the uncertainty in the free-electron g factor, and partially to our neglect of small nuclear mass correction terms and higher-order (α^4) terms. The ratio $g_J\,(\mathrm{He},\,2\,^3S_1)/g_J(\mathrm{H},\,1\,^2S_{\frac{1}{2}}) = 1-23.212\times10^{-6}$ has been calculated with an estimated uncertainty of 3×10^{-9}, this uncertainty arising from the neglect of nuclear mass corrections and α^4 terms. To this order, no uncertainty should arise from the wave function we have used.

Both results, Eqs. (15) and (16), agree with and improve upon the accuracy of previous theoretical values obtained by V. W. Hughes and co-workers.[6] They also agree with early experiments.[11] However, the most recent and precise experimental determination,[5] $g_J(\mathrm{He},\,2\,^3S_1)/g_J(\mathrm{H},\,1\,^2S_{\frac{1}{2}}) = 1 - (21.6\pm0.5)\times10^{-6}$, disagrees significantly with Eq. (16) above. In fact, this disagreement occurs at the level of terms of order α^2. Although it has been suggested[5] that the neglect of higher-order terms in the theory might be responsible for the disagreement between this recent experimental determination and the theoretical calculations,[6] the radiative correction calculated here, which is of order α^3 and contributes -0.135 ppm to the helium g factor, is not large enough to resolve the discrepancy. Since additional corrections are of higher order than α^3, one can conclude that there exists a basic discrepancy between this experiment and the theory.

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[1] See, for example, *Precision Measurement and Fundamental Constants*, edited by D. N. Langenburg and B. N. Taylor, Natl. Bur. Std. Special Publ. No. 343 (U. S. GPO, Washington, D. C., 1971).

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[8] This convention for the sign of g_J is consistent with that of Ref. 4, and results in a negative g factor for the electron. (Another convention also exists in which g factors are defined to be positive.)

[9] We can make an order-of-magnitude estimate of this term using the value for $\langle\vec{r}_1\cdot\vec{r}_2\rangle$ and other integrals given in Ref. 7: $\langle\vec{r}_1\cdot\vec{r}_2/r_1^3\rangle=\langle r_2\;\cos\omega/r_1^2\rangle\cong\langle r_2\rangle\langle1/r_1^2\rangle\,\langle\cos\omega\rangle\cong\langle r_1\rangle\langle1/r_1^2\rangle \times\langle\vec{r}_1\cdot\vec{r}_2\rangle/\langle r_1\rangle^2=\langle1/r_1^2\rangle\langle\vec{r}_1\cdot\vec{r}_2\rangle/\langle r_1\rangle\cong-0.1\alpha m$, where ω is the angle between $\vec{r}_1$ and $\vec{r}_2$. Then the contribution to the g factor is $-2\alpha(6\times4M_p)^{-1}\times(-0.1\alpha m)\times2\times g_e=g_e\times0.0167\alpha^2 m/M_p \cong g_e\times5\times10^{-10}$, which is negligible.

[9a] All the numerical results presented here are for the ^{4}He isotope. Results for ^{3}He can be calculated easily from Eq. (13). We find $g_j(^3\mathrm{He},\,2\,^3S)/g_j\,(^4\mathrm{He},\,2\,^3S) = 1+2.6\times10^{-9}$ with an uncertainty of 1×10^{-9} due to our neglecting the third line of Eq. (12). This ratio could be calculated more precisely by calculating the neglected terms.

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