High-precision calculation of the isotope shift in the ratio $g_J(^3\mathrm{He}, 2\,^3S_1)/g_J(^4\mathrm{He}, 2\,^3S_1)$

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The isotope shift for the Zeeman g_J-factor ratio, including relativistic corrections of orders α^2, $\alpha^2 m/M$, and α^3, is calculated to high precision using variational wave functions. The finite-mass corrections coming from the mass scaling and from the mass polarization term are treated exactly. The result is $g_J(^3\mathrm{He},\ 2\,^3S_1)/g_J(^4\mathrm{He},\ 2\,^3S_1) = 1 + 2.708\,439\,694\,74(76) \times 10^{-9}$. Our calculation significantly improves the previous theoretical prediction of Barkley and Hegstrom [Phys. Rev. A **14**, 1574 (1976)] for this isotope shift.

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I. INTRODUCTION

The study of the isotope shift for the bound electron g_J-factor ratio of an atom in an S state is of special interest. This is because this isotope shift is directly related to nuclear relativistic finite-mass corrections and comparison with experiment would then test the relativistic motional effects in an atom. Extensive experimental measurements have been made for hydrogenic atoms [1] to a precision of 3×10^{-11}, which have confirmed the theoretical prediction made by Grotch and Hegstrom [2]. For many-electron atoms, Hegstrom [3] studied nuclear mass and anomalous magnetic moment corrections to the Hamiltonian for an atom in an external magnetic field and showed that the magnetic-field dependence of the radiative corrections of $O(\alpha^3)$ vanishes for S states. Grotch and Hegstrom [4] applied Hegstrom's work to the helium atom and calculated the g_J factor for the helium $2\,^3S_1$ state. Then, Barkley and Hegstrom [5] extended Grotch and Hegstrom's formula by including explicitly nuclear finite-mass corrections of order $\alpha^2 m/M$, $\alpha^3 m/M$, and $\alpha^2 m^2/M^2$, and evaluated the isotope shift of the g_J-factor ratio $g_J(^3\mathrm{He}, 2\,^3S_1)/g_J(^4\mathrm{He}, 2\,^3S_1)$. However, in their calculations, the mass polarization effects were completely neglected. In addition, one of the finite nuclear mass corrections of order $\alpha^2 m/M$ is proportional to the integral $\langle \mathbf{r}_1 \cdot \mathbf{r}_2/r_1^3 \rangle$. The integral was first estimated by Grotch and Hegstrom [4] and then calculated by Barkley and Hegstrom [5] using the 50 term configuration-interaction wave function of Birss and Senn [6], but both values are of poor accuracy. Recently, Anthony and Sebastian [7] considered the mass polarization term as a first-order perturbation. However, in the use of the virial theorem $\langle T \rangle = -E$, they did not include the mass polarization operator in T [see Eq. (35) of Ref. [7]]. In fact, T should be understood as a sum of all quadratic terms as one might gather from the discussion of Bethe and Salpeter [8]. The incorrect value of Barkley and Hegstrom for the quantity $\langle \mathbf{r}_1 \cdot \mathbf{r}_2/r_1^3 \rangle$ was also used in their calculations of the g_J factors.

In general, inaccuracy in the value of $\langle \mathbf{r}_1 \cdot \mathbf{r}_2/r_1^3 \rangle$ and insufficiency in the treatment of the mass polarization effects may limit the accuracy of the theoretical prediction for the g_J-factor isotope shift. A precise calculation of this isotope shift will thus become the main objective of this paper.

II. CALCULATIONS

The starting point for evaluating the Zeeman g_J factor for the $2\,^3S_1$ state of helium is, according to Grotch and Hegstrom [4]

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

where the matrix element is evaluated in the state $J = 1, M_J = 1$, H'_Z is the magnetic-field dependent part of the Zeeman Hamiltonian derived by Hegstrom [3], H is the external magnetic field, μ_B is the Bohr magneton. Here Grotch and Hegstrom's convention has been used, in which the g_J factor for the electron is negative. Following Grotch and Hegstrom, we obtain our final expression for the g_J factor of helium in the $2\,^3S_1$ state, accurate to α^3 (in atomic units throughout)

$$\begin{aligned} g_J(2\,^3S_1) = g_e &+ \alpha^2 \left(\frac{g_e}{6} - \frac{2}{3}\right) F_5 \\ &+ \alpha^2 \frac{Z}{3} \left[1 + g_e \left(1 - \frac{m}{M}\right)\right] F_6 \\ &- \alpha^2 \frac{1}{6} (1 + 2\,g_e)\, F_7 - \alpha^2 \frac{Z}{3} \frac{m}{M} g_e F_S\,, \end{aligned} \tag{2}$$

where [9]

$$\begin{aligned} g_e = -2\,[1 &+ \alpha/2\pi - 0.328\,478\,965\,(\alpha/\pi)^2 \\ &+ 1.176\,11\,(\alpha/\pi)^3 + \cdots]\,, \end{aligned} \tag{3}$$

m/M is the electron to nuclear mass ratio, and Z is the atomic number. The matrix elements F_5, F_6, F_7, and F_S are defined by [10]

$$F_5 = \langle 2\,^3S_1 | \nabla_1^2 | 2\,^3S_1 \rangle\,, \tag{4}$$

$$F_6 = \left\langle 2\,^3S_1 \left| \frac{1}{r_1} \right| 2\,^3S_1 \right\rangle\,, \tag{5}$$

TABLE I. Coefficients ε_0, ε_1, and ε_2 for the matrix elements F_5, F_6, F_7, and F_S of helium in $2\,^3S_1$ state (in a.u.).

Term	ε_0	ε_1	ε_2
F_5	−2.175 229 378 236 790 19(67)	0.014 884 260 832(35)	−0.172 482 95(22)
F_6	1.154 664 152 972 107 12(22)	−0.004 832 752 624(17)	0.045 211 92(11)
F_7	0.268 197 855 414 847 530(28)	−0.004 446 749 439 2(47)	0.065 858 197(28)
F_S	−0.063 328 398 29(20)	1.031 234(14)	−0.048(82)

$$F_7 = \left\langle 2\,^3S_1 \left| \frac{1}{r_{12}} \right| 2\,^3S_1 \right\rangle , \tag{6}$$

$$F_S = \left\langle 2\,^3S_1 \left| \frac{\mathbf{r}_1 \cdot \mathbf{r}_2}{r_1^3} \right| 2\,^3S_1 \right\rangle . \tag{7}$$

The necessary matrix elements in Eqs. (4)–(7) were calculated to high precision by the use of variational wave functions constructed from doubled basis sets in Hylleraas coordinates, as described previously [11]. The explicit form for the wave functions is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{ijk} [a^{(1)}_{ijk}\, \chi_{ijk}(\alpha_1, \beta_1) + a^{(2)}_{ijk}\, \chi_{ijk}(\alpha_2, \beta_2)] \pm (\text{exchange}) , \tag{8}$$

with

$$\chi_{ijk} = r_1^i\, r_2^j\, r_{12}^k\, e^{-\alpha r_1 - \beta r_2} \tag{9}$$

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.

In order to exhibit all the nuclear mass terms explicitly, we rescale the Hamiltonian according to $r \longrightarrow (m/\mu)\, r$. Then our Hamiltonian becomes

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} - \frac{\mu}{M}\nabla_1 \cdot \nabla_2, \tag{10}$$

where $\mu = mM/(m+M)$ is the reduced mass. Thus, the matrix element of an operator O whose degree of homogeneity is n with respect to powers of r can be expanded in powers of μ/M according to

$$\langle \Psi | O | \Psi \rangle = (\mu/m)^{-n} [\varepsilon_0 + \varepsilon_1\, (\mu/M) + \varepsilon_2\, (\mu/M)^2 + \cdots] , \tag{11}$$

where Ψ is the wave function of the original Hamiltonian, and $(\mu/m)^{-n}$ is from the mass scaling transformation. The first three coefficients ε_0, ε_1, and ε_2 can be determined through three calculations for three different nuclear masses. Here we choose infinite mass, the mass of ^{3}He, and the mass of ^{4}He. It is obvious that the first coefficient is $\varepsilon_0 = \langle \Psi_\infty | O | \Psi_\infty \rangle$, where Ψ_∞ is the wave function with the infinite nuclear mass. The numerical values of ε_i are listed in Table I. Note that our value for F_S, in the infinite-mass approximation, is −0.063 328 398 29(20) a.u. On the other hand, the Grotch and Hegstrom's estimated value [4] is −0.1 a.u., while Barkley and Hegstrom's value [5] is −0.149 860 a.u., which was expected by them to be accurate to four or five significant figures. Our final results are contained in Table II, together with the existing theoretical values. The second row of Table II is calculated using Eq. (1) of Barkley and Hegstrom's paper [5], with the matrix element F_S replaced by our correct value. It is clear that the mass polarization contributes at 0.6% level and thus cannot be neglected.

Finally, it is also necessary to reexamine how the g_J-factor ratio of $2\,^3S_1$ helium to $1\,^2S_{1/2}$ hydrogen is affected by our results. The expression for the g_J factor of hydrogenic atoms in the $1\,^2S_{1/2}$ state can be found in Ref. [2]. Our results are

$$g_J(^3\mathrm{He}, 2\,^3S_1)/g_J(^1\mathrm{H}, 1\,^2S_{1/2}) = 1 - 23.208\,888 \times 10^{-6} , \tag{12}$$

$$g_J(^4\mathrm{He}, 2\,^3S_1)/g_J(^1\mathrm{H}, 1\,^2S_{1/2}) = 1 - 23.211\,597 \times 10^{-6} , \tag{13}$$

which within 10^{-9} agree with the previous theoretical results of Barkley and Hegstrom [5] and of Anthony and Sebastian [7], and also agree with the best experimental measurement of Keiser and Robinson [12], which is $1 - 23.214(50) \times 10^{-6}$ for $g_J(^4\mathrm{He}, 2\,^3S_1)/g_J(^1\mathrm{H}, 1\,^2S_{1/2})$.

TABLE II. Theoretical value of the isotope shift for the g_J-factor ratio $[g_J(^3\mathrm{He}, 2\,^3S_1)/g_J(^4\mathrm{He}, 2\,^3S_1) - 1] \times 10^9$. In the present work $m/M\,(^3\mathrm{He}) = 1.819\,543\,056 \times 10^{-4}$ and $m/M\,(^4\mathrm{He}) = 1.370\,933\,540 \times 10^{-4}$, $\alpha^{-1} = 137.035\,989\,5(61)$. The errors quoted in our isotope shifts do not include the errors in the fundamental constants.

Theory	Isotope shift
Present work with mass polarization	2.708 439 694 74(76)
Present work without mass polarization	2.692 457 812 25
Barkley and Hegstrom [a]	2.830 3
Anthony and Sebastian [b]	2.796 9

[a] Reference [5].
[b] Reference [7].

From the above discussion, it can be seen that the isotope shift is much more sensitive to mass polarization effects and to the matrix element F_S than the g_J-factor ratios of helium to hydrogen.

III. SUMMARY AND CONCLUSIONS

We have performed a high-precision calculation for the isotope shift of the Zeeman g_J-factor ratio for the $2\,^3S_1$ state of helium. For the first time, the finite-mass effects due to the mass scaling and mass polarization, which are proven to be important in the study of isotope shift, have been dealt with exactly. An error in the numerical value of F_S, which has stood for a long time in literature, has been corrected. The only uncalculated terms in the isotope shift are of order $\alpha^4\,[m/M\,(^3\mathrm{He}) - m/M\,(^4\mathrm{He})]$ and higher which are about 0.0001×10^{-9}. Although to the best of our knowledge there are no experimental measurements reported so far for the helium g_J-factor isotope shift, our theoretical prediction may become a timely challenge to experimentalists.

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