Accurate determination of ^{6,7}Li nuclear magnetic moments

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We report an accurate determination of the nuclear magnetic dipole moments of ^{6,7}Li from the measured ratio of the nuclear and the electron g-factors in atomic Li. The obtained results significantly improve upon the literature values and stress the importance of reliable theoretical calculations of the nuclear shielding corrections.

Standard tabulations of the nuclear moments [1, 2] often rely on data derived from the nuclear magnetic resonance measurements. In order to extract the magnetic moment of bare nuclei from these experiments, one has to correct for the so-called chemical shifts originating from the surrounding electrons and neighbouring atoms. Such shifts are difficult to calculate reliably, which often leads to significant systematic uncertainties in the literature data on nuclear magnetic moments. As an example, the so-called "bismuth hyperfine puzzle" [3, 4] was recently resolved [5] and traced back to the previously underestimated uncertainty of the correction due to the chemical surrounding in the determination of the nuclear magnetic moment of bismuth.

Much more accurate determinations of nuclear magnetic moments can be performed from measurements of the combined Zeeman and hyperfine structure of atomic levels. The nuclear and electron g factors in atomic systems can be nowadays calculated within QED to a very high accuracy, with reliable estimations of uncertainties due to uncalculated higher-order effects. High-precision determinations of nuclear magnetic moments were recently reported for deuterium and tritium [6], ^{3}He [7], and ^{9}Be [8]. In this work we perform an accurate determination of the nuclear magnetic dipole moments of ^{6,7}Li from measured ratios of the nuclear and the electron g-factors [9]. The nuclear moment of ^{7}Li is of particular importance since it is used as a reference in determinations of magnetic moments of unstable ^{8,9,11}Li isotopes [10–12]. Improved values of the nuclear magnetic moments of Li isotopes are also needed in view of continuing efforts [13–15] to determine values of the so-called effective Zemach radii characterizing the magnetization distribution over the nuclear volume from hyperfine-structure measurements.

Magnetic g-factors of an atomic system are defined through the effective interaction with the magnetic field

$$H = -\frac{e}{2\,m_e}\,g_J\,\vec{J}\cdot\vec{B} - \frac{e}{2\,m_p}\,g_I\,\vec{I}\cdot\vec{B} + A\,\vec{J}\cdot\vec{I}\,, \qquad (1)$$

where $\vec{B}$ is the external magnetic field, $\vec{I}$ and $\vec{J}$ are the total angular momentum of the nucleus and electrons, respectively, g_I and g_J are the g factors of the nucleus and electrons, respectively, m_p and m_e are the mass of the proton and the electron, respectively, e is the elementary charge, and A is hyperfine constant. We note that our definition of the nuclear g-factor contains m_p, whereas a different definition $g'_I = (m_e/m_p)\,g_I$ is also used in the literature.

The nuclear g-factor g_I of an atom is connected to the free-nucleus g-factor g_N by the shielding constant σ,

$$g_I = g_N\,(1-\sigma)\,, \qquad (2)$$

which can be accurately calculated by the atomic theory. For a light atom, the shielding constant σ is effectively described by a double expansion in powers of the fine-structure constant α and the electron-to-nucleus mass ratio m_e/m_N,

$$\sigma = \alpha^2\,\sigma^{(2)} + \alpha^4\,\sigma^{(4)} + \alpha^2\,\frac{m_e}{m_N}\sigma^{(2,1)} + \ldots\,. \qquad (3)$$

The first term of this expansion, $\sigma^{(2)}$, is obtained from the Ramsey nonrelativistic theory of the magnetic shielding [16]. For atomic systems it has a very simple form

$$\sigma^{(2)} = \frac{1}{3}\sum_a \left\langle \frac{1}{r_a} \right\rangle, \qquad (4)$$

where the summation over a runs over all electrons. This matrix element was calculated with a high accuracy by Yan [17, 18] with the Hylleraas basis set. The result for the leading-order shielding contribution (in the infinite nuclear mass limit) for Li is

$$\alpha^2\,\sigma^{(2)} = 101.499\times 10^{-6}\,. \qquad (5)$$

The relativistic shielding correction, $\sigma^{(4)}$, was recently calculated for helium [7, 19]. For Li, there have been no calculations of this contribution so far. Here, we estimate this correction on the basis of known hydrogenic result. For hydrogenic ions, the relativistic shielding constant can be derived analytically in a closed form [20, 21]. After expanding in $Z\alpha$, the hydrogenic (H) result reads

$$\sigma_{\rm H} = \frac{\alpha\,(Z\alpha)}{3\,n^2}\left[1 + \frac{132\,n-35}{36\,n^2}\,(Z\alpha)^2\right] + O(\alpha^6), \qquad (6)$$

where n is the principal quantum number. A straightforward application of this formula to the ground state of Li leads to the following result in the leading order in α:

$$\alpha^2\,\sigma^{(2)} = \frac{\alpha^2}{3}\left[2\,Z + \frac{Z-2}{2^2}\right] = 111\times 10^{-6}\,, \qquad (7)$$

TABLE I: The magnetic moments of light nuclei.

Element	μ/μ_N	Ref.
^{2}H	0.857 438 233 8 (26)	[6]
^{3}H	2.978 962 465 0 (59)	[6]
^{3}He	−2.127 625 350 0 (17)	[7, 24]
^{6}Li	0.822 044 63 (37)	this work
	0.822 045 7 (50)	[25]
	0.822 043 (3)	[26]
	0.822 047 3 (6)	[9], as quoted in [2]
	0.822 567 (3)	[27], as quoted in [2]
^{7}Li	3.256 416 19 (57)	this work
	3.256 418 (20)	[25]
	3.256 407 (12)	[26]
	3.256 427 (2)	[9], as quoted in [2]
	3.256 462 5 (4)	[27], as quoted in [2]
^{9}Be	−1.177 431 59 (3)	[8]

which deviates only by 10% from the exact result of Eq. (5). Such an agrement is not surprising because mostly core electrons contribute to σ, and for Li they do not differ significantly from the hydrogenic case. Next, we apply Eq. (6) to estimate the relativistic shielding correction for the helium atom. The second term of the α expansion of Eq. (6) yields

$$\alpha^4\,\sigma^{(4)}_{\rm He} = 2\,\alpha^4\,Z^3\,\frac{97}{108}\,, \tag{8}$$

With $Z = 2$, it gives 0.040 750, which is by 30% smaller than the exact result $\alpha^4\,\sigma^{(4)}_{\rm He} = 0.052\,663\,1$ [7, 19]. Analogously, we estimate the relativistic shielding correction for Li as

$$\alpha^4\,\sigma^{(4)} = \frac{\alpha^4}{3}\left[2\,Z^3\,\frac{97}{36} + (Z-2)^3\,\frac{229}{576}\right]. \tag{9}$$

and ascribe a 30% accuracy to this approximation. We thus obtain

$$\alpha^4\,\sigma^{(4)} = 0.138\,(41)\times 10^{-6}. \tag{10}$$

The last potentially important correction to σ is the one due to the finite nuclear mass. It is given by the formula [22]

$$\sigma^{(2,1)} = \frac{1}{3}\left\langle\sum_a \frac{1}{r_a}\,\frac{1}{(E-H)'}\,p_N^2\right\rangle + \frac{1}{3}\,\frac{(1-\tilde g_N)}{Z\,\tilde g_N}\,\langle p_N^2\rangle + \frac{1}{3}\left\langle\left(\vec r_1\times\vec p_2 + \vec r_2\times\vec p_1\right)\frac{1}{(E-H)}\sum_a \frac{\vec r_a}{r_a^3}\times\vec p_a\right\rangle, \tag{11}$$

where $\vec p_N = -\sum_a \vec p_a$, and

$$\tilde g_N = \frac{m_N}{Z\,m_p}\,\frac{\mu}{\mu_N}\,\frac{1}{I}\,. \tag{12}$$

Since $\sigma^{(2,1)}$ is small, it does not need to be calculated accurately. We therefore neglect the so-called mass-polarization part $\sum_{a>b}\vec p_a\cdot\vec p_b$ in the first and the second term in Eq. (11) and neglect the third term completely. After these simplifications, we obtain the approximate form of the finite nuclear-mass correction as

$$\sigma^{(2,1)} \approx -\frac{1}{3}\left\langle\sum_a\frac{1}{r_a}\right\rangle - \frac{2}{3}\,\frac{(1-\tilde g_N)}{Z\,\tilde g_N}\,E, \tag{13}$$

where $E = -7.478\,060\,323$ is the nonrelativistic energy of Li in atomic units [23]. The numerical results for the recoil contribution are small but not negligible,

$$\alpha^2\,\frac{m_e}{m_N}\sigma^{(2,1)} \approx \begin{cases} -0.012\times 10^{-6}\,, & \text{for } ^6\text{Li},\\ -0.013\times 10^{-6}\,, & \text{for } ^7\text{Li}. \end{cases} \tag{14}$$

All other corrections to the shielding constant in Li are much smaller and can be neglected on the level of our present interest. Finally, our total values for the shielding constant are

$$\sigma = \begin{cases} 101.62\,(4)\times 10^{-6}\,, & \text{for } ^6\text{Li}\\ 101.62\,(4)\times 10^{-6}\,, & \text{for } ^7\text{Li}\,. \end{cases} \tag{15}$$

The uncertainty of these values comes from the estimate of the relativistic correction; this is the factor limiting the accuracy of our determination of nuclear moments.

The electron g factor in Li was calculated by Yan in Refs. [28, 29]. Recently, Shabaev et al. [30] corrected the nuclear recoil part of Yan's calculation. Using Yan's values for the α^2 and α^3 corrections and the nuclear recoil values from Ref. [30], we obtain

$$\frac{g_J}{g_e} - 1 = \begin{cases} -9.124\,99\,(17)\times 10^{-6}\,, & \text{for } ^6\text{Li},\\ -9.125\,19\,(15)\times 10^{-6}\,, & \text{for } ^7\text{Li}, \end{cases} \tag{16}$$

where g_e is the free-electron g factor. The uncertainties of the above values come from the estimated errors of numerical computation in Ref. [30].

We are now ready to determine the nuclear magnetic moments of ^{6,7}Li. They are obtained from the measured ratio of the nuclear and electron g factors [9],

$$g'_I/g_J = \begin{cases} -2.235\,697\,8(10)\times 10^{-4}\,, & \text{for } ^6\text{Li},\\ -5.904\,271\,9(10)\times 10^{-4}\,, & \text{for } ^7\text{Li}, \end{cases} \tag{17}$$

by means of the formula

$$\frac{\mu}{\mu_N} = g_N\,I = \frac{g'_I}{g_J}\,\frac{g_J}{g_e}\,\frac{g_e}{(1-\sigma)}\,\frac{m_p}{m_e}\,I\,. \tag{18}$$

By using the values for the shielding constant σ and the electron g-factor g_J as summarized above and the free electron g-factor and physical constants from [31, 32], we obtain the results for the nuclear magnetic moments of ^{6,7}Li as presented in Table I.

The comparison with the literature data given in Table I shows significant deviations of the present nuclear magnetic moments from those tabulated in Ref. [2]. The reason is that the previous tabulations typically ignored uncertainties associated with theoretical calculations of diamagnetic corrections. This problem has been recognized and addressed in the updated tabulation [26]. In particular, for ^{6,7}Li, the nuclear moments from Ref. [26] have much larger uncertainties than previously and are in agreement within the present values.

The improved values of the nuclear magnetic moments influence the determinations of the Zemach radii r_Z reported in Refs. [13, 14]. Specifically, the shift of our values of nuclear magnetic moments as compared to those of Ref. [2] leads to a change of r_Z by 0.02 fm for ^{6}Li and 0.03 fm for ^{7}Li, which is comparable with the claimed uncertainties of the r_Z values in Refs. [13, 14]. The most recent values of the effective Zemach radii are $\tilde{r}_z(^6\mathrm{Li}) = 2.39(2)$ fm, and $\tilde{r}_z(^7\mathrm{Li}) = 3.33(3)$ fm [15].

In summary, we have determined the nuclear magnetic dipole moments of ^{6,7}Li with an improved precision as compared to the literature values. Our work indicates the importance of reliable estimations of uncertainties in the calculation of corrections to the nonrelativistic nuclear magnetic shielding.

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