Accurate determination of Be magnetic moment

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The determination of the magnetic moment of ^{9}Be from the measured ratio of the nuclear to the electron g-factors g_I/g_J in $^9\mathrm{Be}^+$ is presented. The obtained result $\mu(^9\mathrm{Be}) = -1.177\,431\,59(3)\,\mu_N$ is two orders of magnitude more accurate than the presently accepted value.

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The determination of nuclear magnetic moments from the atomic hyperfine splitting is significantly affected by nuclear structure corrections. These corrections include finite distribution of the charge and the magnetization, and also the nuclear polarizability, the last one is not negligible even for light nuclei [1]. Whereas the charge distribution is, in general sufficiently well known, the magnetic formfactor and polarizability are difficult to access experimentally. For this reason, theoretical predictions for the hyperfine splitting are uncertain due to the difficult to estimate nuclear structure effects. If the nuclear magnetic moment can be obtained independently by other means, from the difference between experimental hyperfine splitting and accurate calculations assuming point nucleus, one can determine the nuclear structure contribution and thus test predictions of various nuclear models, expecially interesting for halo nuclei [2]. Very similar idea was applied recently for the determination of nuclear charge radii from the measured value of the isotope shift in H, He, Li and Be, see for example the most recent work in [3].

In this work we demonstrate, that nuclear magnetic moment can be accurately determined from the measurement of Zeeman hyperfine splittings. More precisely, we obtain the ^{9}Be magnetic moment using the measured value [4] of the ratio of the nuclear to the electron g-factors in $^9\mathrm{Be}^+$, which is

$$g'_I/g_J = 2.134\,779\,853(2)\times 10^{-4}. \tag{1}$$

A slightly different result was obtained in [5]

$$g'_I/g_J = 2.134\,780\,33(28)\times 10^{-4}. \tag{2}$$

The difference according to Authors of [5] is probably due to quadratic dependence of this ratio on the magnetic field B in this later result. Therefore for the determination of the nuclear magnetic moment we will use the first more accurate result.

Magnetic g-factors are defined through effective interaction with the magnetic field

$$H = -\frac{e}{2\,m_e}\,g_J\,\vec J\cdot\vec B - \frac{e}{2\,m_p}\,g_I\,\vec I\cdot\vec B + A\,\vec J\cdot\vec I. \tag{3}$$

For the coupling of the nuclear spin with $\vec B$ one introduces the following related g-factor

$$-\frac{e}{2\,m_p}\,g_I\,\vec I\cdot\vec B = -\frac{e}{2\,m_e}\,g'_I\,\vec I\cdot\vec B \tag{4}$$

which is present in Eqs. (1, 2).

In order to obtain the accurate value of the nuclear magnetic moment $\mu(^9\mathrm{Be})$ one needs to calculate the shielding constant $\sigma(^9\mathrm{Be}^+)$ and the bound electron g-factor $g_J(^9\mathrm{Be}^+)$. The shielding constant is defined by $H = -\vec\mu\cdot\vec B\,(1-\sigma)$, what for the g-factor means

$$g_I = g_N\,(1-\sigma), \tag{5}$$

where g_N is a free nucleus g-factor. For a specified atom σ is a function of the fine structure constant α and depends also on the electron-nucleus mass ratio. Since this ratio is very small, for ^{9}Be it is about $6.1\,10^{-5}$ [6], σ can be expanded in a power series in m_e/m_N. Regarding dependence on α, for the small nuclear charge such as $Z = 4$ the expansion in α is also well convergent. Therefore, one has for σ a double series expansion

$$\sigma = \sigma\Big(\alpha, \frac{m_e}{m_N}\Big) = \alpha^2\,\sigma^{(2)} + \alpha^4\,\sigma^{(4)} + \alpha^2\,\frac{m_e}{m_N}\sigma^{(2,1)} + \ldots \tag{6}$$

The first term of this expansion, $\sigma^{(2)}$, is obtained from the Ramsey nonrelativistic theory [7] of the magnetic shielding and for atomic systems takes the very simple form

$$\sigma^{(2)} = \frac{1}{3}\,\sum_a\Big\langle\frac{1}{r_a}\Big\rangle. \tag{7}$$

We calculate this matrix element using the Hylleraas basis set with the result (in the infinite nuclear mass limit)

$$\sum_a\Big\langle\frac{1}{r_a}\Big\rangle = 7.973\,888\,856\,998\,30(3), \tag{8}$$

and obtain the following nonrelativistic shielding constant

$$\alpha^2\,\sigma^{(2)} = 141.540\,10^{-6}. \tag{9}$$

The number of digits in Eq. (8) is more than sufficient, but we demonstrate here, that theoretical calculations of $\sigma^{(2)}$ are accurate enough to make use of the high precision experimental value for the g-factor ratio, such as that in Eq. (1). The relativistic corrections are much more difficult in the calculations. There are no published results for $^9\mathrm{Be}^+$. In fact, most calculations correspond to chemical shifts, but not to the absolute shielding constant. The only known accurate calculation of $\sigma^{(4)}$ was performed recently for ^{3}He in Ref. [8]. Here, we estimate this correction on the basis of $1/Z$ expansion. The

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analytic result for the relativistic shielding constant in hydrogenic ions was obtained in Ref. [9]. The first terms in the expansion in $Z\,\alpha$ are

$$\sigma_H = \frac{\alpha\,(Z\,\alpha)}{3\,n^2}\left[1+\frac{132\,n-35}{26\,n^2}\,(Z\,\alpha)^2\right]+O(\alpha^6), \quad (10)$$

where n is the principal quantum number. The naive application of this formula to the ground state of Be^+

$$\alpha^2\,\sigma_H^{(2)} = \frac{\alpha^2}{3}\left[2\,Z+\frac{Z-2}{2^2}\right] = 150.879\,10^{-6} \quad (11)$$

with $Z=4$, agrees well, within few %, with the accurate value in Eq. (9). It is because mostly core electrons contribute to σ, and for Be^+ they do not differ significantly from the hydrogenic ones. We use therefore the next term of the expansion in Eq. (10) to obtain the estimate of the relativistic correction

$$\alpha^4\,\sigma_H^{(4)} = \frac{\alpha^4}{3}\left[2\,Z^3\,\frac{97}{36}+(Z-2)^3\,\frac{229}{576}\right]\approx 0.33\,10^{-6}. \quad (12)$$

We assume 10% accuracy of this results for Be^+ and thus obtain

$$\alpha^4\,\sigma^{(4)} = 0.33(3)\,10^{-6}. \quad (13)$$

The last potentially important correction to σ is due to the finite nuclear mass. It is given by the formula [10]

$$\sigma^{(2,1)} = \frac{1}{3}\left\langle\sum_a \frac{1}{r_a}\,\frac{1}{(E-H)'}\,p_N^2\right\rangle+\frac{1}{3}\,\frac{(1-\tilde g_N)}{Z\,\tilde g_N}\,\langle p_N^2\rangle + \frac{1}{3}\left\langle\left(\vec r_1\times\vec p_2+\vec r_2\times\vec p_1\right)\frac{1}{(E-H)}\sum_a \frac{\vec r_a}{r_a^3}\times\vec p_a\right\rangle, \quad (14)$$

where the nuclear spin $I=3/2$ for ${}^9\mathrm{Be}$, $\vec p_N = -\sum_a \vec p_a$,

$$\tilde g_N = \frac{m_N}{Z\,m_p}\,\frac{\mu}{\mu_N}\,\frac{1}{I} = -1.755\,335(5), \quad (15)$$

and the magnetic moment μ

$$\mu = -1.177\,432(3)\,\mu_N \quad (16)$$

is the presently accepted value for ${}^9\mathrm{Be}$ nucleus [11, 12]. Since $\sigma^{(2,1)}$ is small, it does not need to be calculated accurately, we neglect the so called mass polarization $\sum_{a>b}\vec p_a\cdot\vec p_b$ in the first and the second term in Eq. (14), and neglect the third term completely. Thus the approximate form of the finite nuclear mass correction is

$$\sigma^{(2,1)} \approx -\frac{1}{3}\left\langle\sum_a\frac{1}{r_a}\right\rangle-\frac{2}{3}\,\frac{(1-\tilde g_N)}{Z\,\tilde g_N}\,E, \quad (17)$$

where

$$E = -14.324\,763\,176\,784(11) \quad (18)$$

is the nonrelativistic energy of ${}^9\mathrm{Be}^+$ in atomic units [13]. The numerical value for the recoil contribution

$$\alpha^2\,\frac{m_e}{m_N}\sigma^{(2,1)} \approx -0.021\,10^{-6}, \quad (19)$$

is small but not negligible. There is no other significant correction to the shielding constant, including the finite nuclear size. Therefore, our value for the total shielding constant, according to Eq. (6) is

$$\sigma = 141.85(3)\,10^{-6}, \quad (20)$$

where the uncertainty comes from the estimate of relativistic corrections, and this limits the accuracy of present determination of the nuclear magnetic moment.

Considering the electron g-factor, it was calculated for ${}^9\mathrm{Be}^+$ with high numerical precision by Yan in [14]

$$\frac{g_J}{g_e}-1 = -28.554\,814(1)\,10^{-6}. \quad (21)$$

This result includes relativistic α^2 and QED α^3 terms, but does not include higher order α^4 corrections. They are known only for hydrogenic systems [15]

$$g = 2-\frac{2}{3}\,\frac{(Z\,\alpha)^2}{n^2}+\left(\frac{1}{2\,n}-\frac{2}{3}\right)\frac{(Z\,\alpha)^4}{n^3}+O(Z\,\alpha)^6. \quad (22)$$

The application of this formula to the leading relativistic correction for the valence electron in ${}^9\mathrm{Be}^+$ gives

$$\alpha^2\,\frac{g^{(2)}}{g^{(0)}} = -\frac{1}{3}\,\frac{(Z-2)^2\alpha^2}{4} = -17.75\,10^{-6} \quad (23)$$

a result which is 40% smaller than the correct one in Eq. (21). For analogous estimate of the higher order correction

$$\alpha^4\,\frac{g^{(4)}}{g^{(0)}} = -0.0012(12)\,10^{-6}, \quad (24)$$

we assume 100% uncertainty and thus

$$\frac{g_J}{g_e}-1 = -28.556\,(1)\,10^{-6}. \quad (25)$$

This uncertainty is however, much too small to play a role in the presented determination of the nuclear magnetic moment.

We are now ready to obtain $\mu({}^9\mathrm{Be})$. For this one needs the free electron g-factor, that is known to a very high accuracy [16]

$$g_e/2 = -1.001\,159\,652\,180\,73(28), \quad (26)$$

and all other physical constants are taken from [17]. The resulting magnetic moment is

$$\begin{aligned}\mu &= g_N\,I\,\mu_N\\ &= \frac{g_I'}{g_J}\,\frac{g_J}{g_e}\,\frac{g_e}{(1-\sigma)}\,\frac{m_p}{m_e}\,I\,\mu_N\\ &= -1.177\,431\,59(3)\,\mu_N,\end{aligned} \quad (27)$$

where the uncertainty comes from the relativistic correction to the shielding constant σ. Its calculation would allow for another order of magnitude improvement in the ${}^9\mathrm{Be}$ magnetic moment. Inspite of this, even now it is one of the most accurately known magnetic moment among all elements.

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