Observation of the Nuclear Magnetic Octupole Moment of $^{87}$Rb from Spectroscopic Measurements of Hyperfine Intervals

Vladislav Gerginov, Carol E. Tanner and W.R. Johnson
Department of Physics, 225 Nieuwland Science Hall, University of Notre Dame, Notre Dame IN 46556

The magnetic octupole moment of $^{87}$Rb is determined from hyperfine intervals in the $5p\,^2P_{3/2}$ state measured by Ye et al. [Opt. Lett. 21, 1280 (1996)]. Hyperfine constants $A = 84.7189(22)$ MHz, $B = 12.4942(43)$ MHz, and $C = -0.12(99)$ kHz are obtained from the published measurements. The existence of a significant value for $C$ indicates the presence of a nuclear magnetic octupole moment $\Omega$. Combining the hyperfine constants with atomic structure calculations, we obtain $\Omega = -0.58(39)\,\mu_N$. Second-order corrections arising from interaction with the nearby $5p\,^2P_{1/2}$ state are found to be insignificant.

PACS numbers: 21.10.Ky, 32.10.Fn, 42.62.Fi

Keywords: nuclear moments, hyperfine structure, laser spectroscopy

I. INTRODUCTION

We report values of the nuclear magnetic octupole moment of $^{87}$Rb determined from measured hyperfine intervals. During an earlier investigation of the hyperfine structure of atomic $^{133}$Cs [1], we discovered existing measurements of the hyperfine structure of the $5p\,^2P_{3/2}$ state of $^{87}$Rb ($I = 3/2$, $F = 0, 1, 2, 3$) by Ye et al. [2] with a frequency resolution of several kHz. The measured hyperfine intervals $\Delta W_F = W_F - W_{F-1}$ are shown in Fig. 1. These intervals were decomposed in terms of nuclear magnetic dipole and electric quadrupole coupling coefficients ($A$ and $B$) in Ref. [2] and the resulting values for $A$ and $B$ are given in the first row of Table I. However, for an atomic state with angular momentum $J \geq 3/2$, there also exists a coupling between the nuclear magnetic octupole moment and the electronic state, provided $I \geq 3/2$. Precision measurements of the three hyperfine intervals in $^{87}$Rb are sufficient to determine three hyperfine constants $A$, $B$ and $C$, representing the interaction of the nuclear magnetic dipole moment $\mu_I$, electric quadrupole moment $Q$, and magnetic octupole moment $\Omega$, respectively, with the atomic electrons. We combine the coefficient $C$, determined herein, with atomic structure calculations for neutral $^{87}$Rb to determine the nuclear octupole moment. The purpose of the present paper is to determine the previously unknown nuclear magnetic octupole moment of $^{87}$Rb, not to discuss the experimental work by Ye et al.

The (unperturbed) hyperfine structure intervals of an atom having a single electron outside closed shells and $I = J = 3/2$ is given in terms of the hyperfine constants $A$, $B$ and $C$ by [3]

$$\Delta W_3 = 3A + B + 8C \tag{1}$$
$$\Delta W_2 = 2A - B - 28C \tag{2}$$
$$\Delta W_1 = A - B + 56C. \tag{3}$$

Inverting these equations leads to the values of $A$, $B$ and $C$ given in the second row of Table I.

II. SEMI-EMPIRICAL ANALYSIS

With the aid of approximations developed by Casimir [4], semi-empirical estimates for the hyperfine coupling constants can be expressed in terms of the nuclear moments $\mu_I$, $Q$, and $\Omega$ of $^{87}$Rb. To evaluate the hyperfine constants empirically, we start from the nonrelativistic expressions for $A$, $B$ and $C$ [3, Chap. VIII], which can be written

$$A(5p_{3/2}) = \mu_I(\mu_N)\frac{16}{45} \left( \frac{1}{r^7} \right)_{5p} F \times 95.4107 \text{ MHz} \tag{4}$$
$$B(5p_{3/2}) = Q(b) \frac{2}{5} \left( \frac{1}{r^3} \right)_{5p} R \times 234.965 \text{ MHz} \tag{5}$$
$$C(5p_{3/2}) = \Omega(\mu_N b) \frac{2}{35} \left[ \frac{R_{5p}^2(r)}{r^4} \right]_0 T \times 3.40718 \text{ Hz.} \tag{6}$$

The atomic matrix elements in Eqs. (4-6) are expressed in atomic units. In Eq. (6), $R_{5p}(r)$ is the radial wave function.
TABLE I: Hyperfine coupling constants $A$, $B$ and $C$ from
measured hyperfine intervals of $^{87}$Rb $5p^2P_{3/2}$. First row:
results obtained by Ye et al. [2], second row: present analysis,
third row: semi-empirical estimates, fourth row: MBPT results.
In the semi-empirical and MBPT calculations, we use
$\mu_1 = 2.7516\mu_N$ from Raghavan [6] and $Q = 133.5(5)$ mb from
Pyykko [3]. $\Omega$ is expressed in $\mu$eV.

|          | $A$ (MHz) | $B$ (MHz) | $C$ (kHz) |
|----------|-----------|-----------|-----------|
| Ref. [2] | 84.7185(20) | 12.4965(37) |           |
| Present Work | 84.7189(22) | 12.4942(43) | -0.12(09) |
| Semi-empirical | 91.4 | 12.5 | 0.293 $\Omega$ |
| MBPT     | 83.0 | 12.6 | 0.206 $\Omega$ |

function of the $5p$ state and, again, atomic quantities are
expressed in atomic units. The factors $F$, $R$, $T$ in the
above equations account for relativistic effects. With aid
of the [Casimir] approximations, we write

$$\left\langle \frac{1}{r^3} \right\rangle_{np} \approx \frac{Z^2 \pi}{3(n^*)^3} \left( 1 - \frac{\sigma r}{dn} \right) = 0.95983 a_0^{-3}$$ (7)

$$\left[ \frac{R_{2p}^2(r)}{r^4} \right] \approx \frac{4Z^2 \pi}{9(n^*)^3} \left( 1 - \frac{\sigma r}{dn} \right) = 1393.68 a_0^{-5}.$$ (8)

In the above expressions, $Z = 37 - 4 = 33$ is the effective
nuclear charge [3, p. 166], $Z_i = 1$ is the ionic charge, $n^*$
is the effective quantum number of the $5p_{3/2}$ state, and
$\sigma$ is the quantum defect. From Van Wijngaarden [5],
we find $n^* = 2.293$ and $\sigma r/ndn = -0.052$, for the $5p_{3/2}$
state of Rb. Using the values $\mu_1 = 2.7516\mu_N$ [6] and
$Q = 0.1335 \, b$ [7] for $^{87}$Rb, we obtain

$$A(5p_{3/2}) \approx 89.6 \, F \, MHz$$ (9)

$$B(5p_{3/2}) \approx 12.0 \, R \, MHz$$ (10)

$$C(5p_{3/2}) \approx 0.271 \, T \, \Omega \, kHz.$$ (11)

We estimate the relativistic correction factors $F$, $R$, $T$ by
comparing relativistic and nonrelativistic Hartree-Fock
(HF) calculations of $A$, $B$ and $C$. In this way, we obtain
$F = 1.02$, $R = 1.04$, and $T = 1.08$. The semi-empirical
values listed in Table I include these relativistic corrections.
As seen from the table, the semi-empirical value for $A$ differs from experiment by 8%, while the value of $B$ differs by less than 0.1%.

III. RELATIVISTIC MANY-BODY ANALYSIS

In Ref. [8], a relativistic many-body method, referred
to as the SD approximation, in which single and double
excitations of Dirac-Hartree-Fock wave functions are itera-
ted to all orders in perturbation theory, was used to
predict magnetic-dipole hyperfine constants for low-lying
states of alkali-metal atoms to within a few percent.
The SD value for the magnetic-dipole hyperfine constant of
the $5p_{3/2}$ state of $^{85}$Rb from [8] is $A = 24.5$ MHz. This
value is scaled by the ratio

$$\frac{g_I[^{87}\text{Rb}]}{g_I[^{85}\text{Rb}]} = \frac{2.7516/(3/2)}{1.3534/(5/2)} = 3.3885$$

giving $A = 83.0$ MHz for the $5p_{3/2}$ state of $^{87}$Rb shown in
the fourth row of Table I. The all-order method described
in [8] was used here to obtain $B/Q = 94.16$ MHz and
$C/\Omega = 0.206$ kHz, leading to the values of $B$ and $C$ listed
in the fourth row of Table I. The theoretical uncertainty
in these values is estimated to be 2%.

Experimental values of the nuclear moments are listed
in the first row of Table III. By comparing the all-order
SD values of $A/\mu_I$ and $B/Q$ with the experimental values
of $A$, $B$ and $C$ shown in the second-row of Table I, we
obtain the MBPT values of nuclear moments $\mu_1$, $Q$ given
in the second row of Table I. The values of $\mu_1$ and $Q$
determined in this way agree to within 2% with precise
measurements. Comparing the theoretical value of $C/\Omega$
with the experimental value of $C$ given in the second row
of Table III leads to the principal prediction of the present
paper: $\Omega = -0.58(39) \, \mu_N$.

IV. ESTIMATING NUCLEAR MOMENTS

It is of interest to compare values of nuclear moments
inferred from atomic structure calculations with values
obtained directly from nuclear shell-model calculations.
In the extreme shell model [9], properties of $^{87}$Rb can
be described assuming a single valence nucleon moving
around an inert core. According to Schwartz [10], the
shell-model predictions for the nuclear moments $\mu_1$, $Q$
and $\Omega$ are:

$$\mu_1 = \mu_N I \times \left\{ \begin{array}{ll} g_L + (g_S - g_L)/(2I), & I = L + 1/2 \\ g_L - (g_S - g_L)/(2I + 1), & I = L - 1/2 \end{array} \right.$$ (12)

$$Q = -\frac{2I - 1}{2I + 2} g_L \langle r^2 \rangle$$ (13)

$$\Omega = \frac{2}{3} \mu_N \left( \frac{2I - 1}{2I + 4} \right) \langle r^2 \rangle \times \left\{ \begin{array}{ll} (I + 2)(I - 3/2)g_L + g_S, & I = L + 1/2 \\ (I - 1)(I + 5/2)g_L - g_S, & I = L - 1/2 \end{array} \right.$$ (14)

For $^{87}$Rb, the unpaired $p_{3/2}$ proton has total angular
momentum $I = 3/2$, orbital angular momentum $L = 1$, and
spin angular momentum $S = 1/2$. The proton spin gyro-
magnetic ratio is $g_S = 5.585694701(56)$ [11] and the
orbital gyromagnetic ratio is $g_L = 1$. Using the value of
the mean-squared nuclear radius $\langle r^2 \rangle = 0.180 \, b$ from
[12], we obtain the values of the three nuclear moments
given in the third row of Table III. Comparing the shell-
model value of $Q$ with the experimental value shown in
and \( \mathbf{18} \) is the \( 5p_{3/2} - 5p_{1/2} \) fine-structure interval. Relativistic many-body calculations carried out in the SD approximation \( \mathbf{8} \) give

\[
\langle 5p_{3/2} | T_1 | 5p_{1/2} \rangle = 22.3 \text{ MHz/}\mu_N
\]

\[
\langle 5p_{3/2} | T_2 | 5p_{1/2} \rangle = 219.6 \text{ MHz/}\mu_b.
\]

The \( 5p \) fine-structure interval in \( ^{87}\text{Rb} \) is \( \Delta E = 7.123,020.80(5) \text{ MHz} \). Combining these values, we find \( \eta = 3.524 \text{ kHz} \) and \( \zeta = 2.916 \text{ kHz} \).

Including second-order corrections, Eqs. \( \mathbf{11,13} \) become

\[
\Delta W_3 = 3A + B + 8C - \frac{1}{20} \eta - \frac{\sqrt{5}}{100} \zeta \tag{19}
\]

\[
\Delta W_2 = 2A - B - 28C + \frac{1}{45} \eta + \frac{2\sqrt{5}}{75} \zeta \tag{20}
\]

\[
\Delta W_1 = A - B + 56C + \frac{1}{36} \eta - \frac{\sqrt{5}}{60} \zeta. \tag{21}
\]

Inverting these equations leads to the following second-order corrections to the previously determined values of \( A, B \) and \( C \) listed in the second row of Table \( \mathbf{II} \) unchanged and insignificantly increase the value of \( B \) to 12.4944(43) MHz.

\section{V. SECOND-ORDER CORRECTIONS}

Second-order hyperfine corrections will modify Eqs. \( \mathbf{II,13} \) and possibly influence the value of \( C \) extracted from these equations. In this section, we investigate the influence of second-order corrections and show that they have a negligible effect on the \( 5p_{3/2} \) hyperfine constants in \( ^{87}\text{Rb} \). The second-order correction to the energy of a state \( |0\rangle \) can be written

\[
W^{(2)} = \sum_n \frac{\langle 0 | H_{\text{hf}} | n \rangle \langle n | H_{\text{hf}} | 0 \rangle}{E_0 - E_n}, \tag{15}
\]

where \( H_{\text{hf}} \) is the hyperfine interaction Hamiltonian. For the case of interest here, \( |0\rangle \) is a particular hyperfine substate of the \( 5p_{3/2} \) state and the sum over states \( |n\rangle \) is restricted to substates of the nearby \( 5p_{1/2} \) state. Only the two substates \( F = 1 \) and \( F = 2 \) of the \( 5p_{3/2} \) states are modified by interaction with the \( 5p_{1/2} \) state. Following the discussion in \( \mathbf{13} \), we find

\[
W_F^{(2)} = \begin{cases} 
\frac{1}{36} \eta - \frac{\sqrt{5}}{60} \zeta & \text{for } F=1 \\
\frac{2}{81} \eta + \frac{\sqrt{5}}{100} \zeta & \text{for } F=2,
\end{cases} \tag{16}
\]

where

\[
\eta = \mu_2^2 \frac{20 \langle 5p_{3/2} | T_1 | 5p_{1/2} \rangle^2}{\Delta E} \tag{17}
\]

\[
\zeta = \mu_1 Q \frac{20 \sqrt{3} \langle 5p_{3/2} | T_1 | 5p_{1/2} \rangle (5p_{3/2} | T_2 | 5p_{1/2} \rangle)}{3 \Delta E}. \tag{18}
\]

The magnetic dipole operator \( T_1 \) and electric quadrupole operator \( T_2 \) in the atomic reduced matrix elements in the numerators of Eqs. \( \mathbf{17} \) and \( \mathbf{18} \) are defined in \( \mathbf{14} \), Chap. V], and the energy denominator \( \Delta E \) in Eqs. \( \mathbf{17} \) and \( \mathbf{18} \) is the \( 5p_{3/2} - 5p_{1/2} \) fine-structure interval. Relativistic many-body calculations carried out in the SD approximation \( \mathbf{8} \) give

\[
\langle 5p_{3/2} | T_1 | 5p_{1/2} \rangle = 22.3 \text{ MHz/}\mu_N
\]

\[
\langle 5p_{3/2} | T_2 | 5p_{1/2} \rangle = 219.6 \text{ MHz/}\mu_b.
\]

The above equations for the second-order corrections are in precise agreement with results for \( ^{87}\text{Rb} \) presented by Beloy and Derevianko in Ref. \( \mathbf{16} \). The second-order corrections leave the experimental values of \( A, B \) and \( C \) listed in the second row of Table \( \mathbf{II} \) unchanged and insignificantly increase the value of \( B \) to 12.4944(43) MHz.

\section{VI. CONCLUSIONS}

In summary, the precise hyperfine measurements of the \( 5p_{3/2} \) hyperfine interval in \( ^{87}\text{Rb} \) by Ye et al. \( \mathbf{2} \) are reanalyzed, allowing for the possibility of a nonvanishing nuclear magnetic octupole moment. Assuming that second-order effects in the hyperfine interaction are negligible, we obtain the values listed in the second row for the hyperfine constants \( A, B \) and \( C \). In particular, we find a nonzero value for \( C = -0.12(09) \text{ MHz} \). Values of \( A/\mu_1, B/Q \) and \( C/\Omega \) are evaluated both empirically and using relativistic all-order methods. The empirical calculations in combination with the experimental measurements lead to values of \( \mu_1 \) and \( Q \) that agree with other measured values to better than 8%, while the all-order calculations combined with the experimental hyperfine constants lead to values of \( \mu_1 \) and \( Q \) that agree with other measurements at the 2% level. With the aid of all-order calculations, we infer the value \( \Omega = -0.58(39) \mu_1 \mu_b \) for the nuclear magnetic octupole moment. This value (together with
the measured value of $Q$) is larger in magnitude and different in sign than the value predicted by the nuclear shell model. We examined the influence of the second-order hyperfine corrections arising from the interaction between the $5p_{3/2}$ state and the neighboring $5p_{1/2}$ state. These corrections are found to make insignificant changes in the values of $A$, $B$ and $C$ extracted from the measurements. Inasmuch as the experimental uncertainties in the values of $C$ and $\Omega$ are relatively large, more precise measurements of the hyperfine intervals would certainly be desirable.

[1] V. Gerginov, A. Derevianko, and C. E. Tanner, Phys. Rev. Lett. 91, 072501 (2003).
[2] J. Ye, S. Swartz, P. Jungner, and J. Hall, Opt. Lett. 21, 1280 (1996).
[3] L. Armstrong Jr, Theory of the Hyperfine Structure of Free Atoms (Wiley-Interscience, New York, 1971), 1st ed.
[4] H. B. G. Casimir, On the Interaction between Atomic Nuclei and Electrons (Freeman, San Francisco, 1963).
[5] W. Van Wijngaarden, J. Quant. Spectrosc. Radiat. Transfer 57, 275 (1997).
[6] P. Raghavan, At. Data Nucl. Data Tables 42, 189 (1989).
[7] P. Pyykkö, Mol. Phys. 99, 1617 (2001).
[8] M. S. Safronova, W. R. Johnson, and A. Derevianko, Phys. Rev. A 60, 4476 (1999).
[9] M. G. Mayer and J. Jensen, Elementary Theory of Nuclear Shell Structure (John Wiley, New York, 1955).
[10] C. Schwartz, Phys. Rev. 97, 380 (1955).
[11] P. Mohr, B. Taylor, and D. Newell, Rev. Mod. Phys. 80, 633 (2008).
[12] T. Beier, P. J. Mohr, H. Persson, and G. Soff, Phys. Rev. A 58, 954 (1998).
[13] K. Beloy, A. Derevianko, and W. R. Johnson, Phys. Rev. A 77, 012512 (2008).
[14] W. R. Johnson, Atomic Structure Theory (Springer, Berlin, 2007).
[15] A. Banerjee, D. Das, and V. Natarajan, Europhy. Lett. 65, 172 (2002).
[16] K. Beloy and A. Derevianko, Phys. Rev. A 78, 032519 (2008).