Comments on the hyperfine structure of the $6p_{3/2}$ state of Cs.

W. R. Johnson
Department of Physics, University of Notre Dame
Notre Dame, IN 46556

March 27, 2004

Abstract

These are working notes of the phenomenology of the $6p_{3/2}$ hyperfine structure in Cs, written to help with the analysis of experimental data.

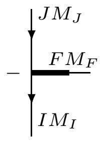
1 Perturbation Expansion

The hyperfine interaction has the form

$$H_{\rm hf} = \sum_{k\lambda} T^{(k)}_{-\lambda}\, M^{(k)}_{\lambda}, \tag{1}$$

Where $T^{(k)}_{-\lambda}$ is an irreducible tensor operator acting in the electron sector and $M^{(k)}_{\lambda}$ is an irreducible tensor operator acting in the nuclear sector. We consider an isolated state, for example the $6p_{3/2}$ state of Cs. We write the wave function of this state as a product of an electronic and nuclear wave function coupled to total angular momentum F:

$$|1\rangle = \sum_{Mm}$$



$$|JM_J\rangle\,|IM_I\rangle\,. \tag{2}$$

The notation used for angular momentum diagrams is that introduced by Lindgren and Morrison [1].

1.1 First-order

The first-order correction to the energy is

$$\begin{aligned} W^{(1)}_F &= \langle 1|H_{\rm hf}|1\rangle \\ &= \sum_k (-1)^{I+J+F} \left\{ \begin{array}{ccc} J & I & F \\ I & J & k \end{array} \right\} \left\langle J\|T^{(k)}\|J\right\rangle \left\langle I\|M^{(k)}\|I\right\rangle , \end{aligned} \tag{3}$$

where we have used

$$\langle n|H_{\rm hf}|1\rangle = \sum_k (-1)^{I+J+F} \left\{ \begin{array}{ccc} J_n & I & F \\ I & J & k \end{array} \right\} \left\langle J_n \| T^{(k)} \| J \right\rangle \left\langle I \| M^{(k)} \| I \right\rangle . \quad (4)$$

The expression for $W_F^{(1)}$ can be rewritten in terms of stretched matrix elements as

$$W_F^{(1)} = \sum_k M(IJ,F;k) \left\langle JJ \| T_0^{(k)} \| JJ \right\rangle \left\langle II \| M_0^{(k)} \| II \right\rangle , \quad (5)$$

where

$$M(IJ,F;k) = \frac{\sqrt{(2I-k)!(2I+k+1)!(2J-k)!(2J+k+1)!}}{(2I)!(2J)!} \times (-1)^{I+J+k} \left\{ \begin{array}{ccc} J & I & F \\ I & J & k \end{array} \right\} . \quad (6)$$

Define the following quantities:

$$\begin{aligned} I_+ &= I(I+1) \\ J_+ &= J(J+1) \\ F_+ &= F(F+1) \\ K &= F_+ - J_+ - I_+ \\ K_+ &= K(K+1). \end{aligned}$$

With this notation, we may write

$$M(IJ,F;1) = \frac{K}{2IJ}, \quad (7)$$

$$M(IJ,F;2) = \frac{3K_+ - 4J_+I_+}{2I(2I-1)J(2J-1)}, \quad (8)$$

$$M(IJ,F;3) = \frac{5K^2(K+4) - 4K[3J_+I_+ - J_+ - I_+ - 3] - 20J_+I_+}{I(2I-1)(2I-2)J(2J-1)(2J-2)}. \quad (9)$$

We now re-express the stretched nuclear matrix elements in terms of conventional nuclear moments:

$$\left\langle II|M^{(1)}|II \right\rangle = \mu \quad (10)$$

$$\left\langle II|M^{(2)}|II \right\rangle = \frac{1}{2}Q \quad (11)$$

$$\left\langle II|M^{(3)}|II \right\rangle = -\Omega. \quad (12)$$

Here, μ is the nuclear magnetic dipole moment, Q is the nuclear electric quadrupole moment, and Ω is the nuclear magnetic octupole moment. Now, we introduce the conventional hyperfine constants a, b, and c:

$$a = \frac{\mu}{IJ}\left\langle JJ|T_0^{(1)}|JJ\right\rangle = \frac{1}{IJ}\left\langle II|M_0^{(1)}|II\right\rangle\left\langle JJ|T_0^{(1)}|JJ\right\rangle \tag{13}$$

$$b = 2Q\left\langle JJ|T_0^{(2)}|JJ\right\rangle = 4\left\langle II|M_0^{(2)}|II\right\rangle\left\langle JJ|T_0^{(2)}|JJ\right\rangle \tag{14}$$

$$c = -\Omega\left\langle JJ|T_0^{(3)}|JJ\right\rangle = \left\langle II|M_0^{(3)}|II\right\rangle\left\langle JJ|T_0^{(3)}|JJ\right\rangle \tag{15}$$

With this notation, we may write the first-order hyperfine energy of a state as

$$\begin{aligned} W_F^{(1)} &= \frac{1}{2}K\,a \\ &+ \frac{3K_+ - 4J_+I_+}{8I(2I-1)J(2J-1)}\,b \qquad (16) \\ &+ \frac{5K^2(K+4) - 4K[3J_+I_+ - J_+ - I_+ - 3] - 20J_+I_+}{I(2I-1)(2I-2)J(2J-1)(2J-2)}\,c\,. \qquad (17) \end{aligned}$$

1.2 Second-order

The second-order correction may be written

$$W_F^{(2)} = \sum_{n\neq 1}\frac{\langle 1|H_{\rm hf}|n\rangle\,\langle n|H_{\rm hf}|1\rangle}{E_1 - E_n}. \tag{18}$$

After angular reduction, this correction can be expressed as

$$\begin{aligned} W_F^{(2)} &= \sum_{n\neq 1}\sum_{kk'}(-1)^{J+J_n+2I+2F}\left\{\begin{array}{ccc} J_n & I & F \\ I & J & k\end{array}\right\}\left\{\begin{array}{ccc} J & I & F \\ I & J_n & k'\end{array}\right\} \\ &\times\frac{\left\langle J_n\|T^{(k)}\|J\right\rangle\left\langle I\|M^{(k)}\|I\right\rangle\left\langle J\|T^{(k')}\|J_n\right\rangle\left\langle I\|M^{(k')}\|I\right\rangle}{E_1 - E_n}. \qquad (19) \end{aligned}$$

For our example of the $6p_{3/2}$ state of Cs, the second-order correction is dominated by the single state $n = 6p_{1/2}$. Moreover, the largest contribution from this state is that associated with the magnetic dipole term $k = k' = 1$. The resulting single perturbing state correction is given by

$$W_F^{(2)} \approx \left\{\begin{array}{ccc} J_n & I & F \\ I & J & 1\end{array}\right\}^2\frac{\left|\left\langle J_n\|T^{(1)}\|J\right\rangle\right|^2\left|\left\langle I\|M^{(1)}\|I\right\rangle\right|^2}{E_1 - E_n}. \tag{20}$$

1.3 Numerical approximations

In this subsection, we estimate the size of the second-order correction by expressing $\left\langle J_n\|T^{(1)}\|J\right\rangle$ in terms of $a_{6p_{3/2}}$ in the nonrelativistic HF limit. The resulting estimate could be improved if necessary using MBPT.

In the one-particle approximation, we may write

$$\left\langle w|T^{(1)}|v\right\rangle = (\kappa_w + \kappa_v)\,\langle -\kappa_w m_w|C_1|\kappa_v m_v\rangle\left(\frac{1}{r^2}\right)_{wv}, \tag{21}$$

where

$$\left(\frac{1}{r^2}\right)_{wv} = \int_0^\infty \frac{dr}{r^2}\left(P_w(r)\,Q_v(r) + Q_w(r)\,P_v(r)\right). \tag{22}$$

In the nonrelativistic approximation, this reduces to

$$\left(\frac{1}{r^2}\right)_{wv} \approx \left(\frac{P_w P_v}{r^2}\right)_{r=0} - \frac{\kappa_w + \kappa_v + 2}{2c}\left\langle \frac{1}{r^3}\right\rangle_{wv} \tag{23}$$

From this, it follows that

$$\begin{aligned}\left\langle 6p_{3/2}, j_v|T^{(1)}|6p_{3/2}, j_v\right\rangle &= -\frac{2\kappa_v(2\kappa_v+2)}{2c}\,\langle j_v\, j_v|C_1|j_v\, j_v\rangle \left\langle \frac{1}{r^3}\right\rangle_{vv} \\ &= \frac{l_v(l_v+1)}{(j_v+1)\,c}\left\langle \frac{1}{r^3}\right\rangle_{vv}\end{aligned} \tag{24}$$

This leads to

$$a_{6p_{1/2}} = \frac{\mu}{I j_v}\frac{4}{3\,c}\left\langle \frac{1}{r^3}\right\rangle_{6p} = \frac{\mu}{c}\,\frac{16}{21}\left\langle \frac{1}{r^3}\right\rangle_{6p} \tag{25}$$

$$a_{6p_{3/2}} = \frac{\mu}{I j_v}\frac{4}{5\,c}\left\langle \frac{1}{r^3}\right\rangle_{6p} = \frac{\mu}{c}\,\frac{16}{105}\left\langle \frac{1}{r^3}\right\rangle_{6p} \tag{26}$$

If the matrix element is evaluated using nonrelativistic HF wave functions and $g_I = 0.73772$, then one obtains

$$a_{6p_{1/2}} = 114.29 \text{ MHz} \tag{27}$$

$$a_{6p_{3/2}} = 22.86 \text{ MHz} \tag{28}$$

The corresponding experimental values are

$$a_{6p_{1/2}} = 291.89 \text{ MHz} \tag{29}$$

$$a_{6p_{3/2}} = 50.275 \text{ MHz} \tag{30}$$

The ratio of the experimental values is 5.8 compared to the ratio 5 for nonrelativistic theory.

Let us consider the off-diagonal matrix element

$$\begin{aligned}\left\langle 6p_{1/2}\|T^{(1)}\|6p_{3/2}\right\rangle &= \frac{\langle 1/2\|C_1\|3/2\rangle}{2c}\left\langle \frac{1}{r^3}\right\rangle_{6p} \\ &= \frac{1}{\sqrt{3}\,c}\left\langle \frac{1}{r^3}\right\rangle_{6p} \qquad (31) \\ &= \frac{105}{16\sqrt{3}}\,\frac{a_{6p_{3/2}}}{\mu} \qquad (32)\end{aligned}$$

We note that

$$\left\langle I\|M^{(1)}\|I\right\rangle = \sqrt{\frac{(I+1)(2I+1)}{I}}\;\mu = \sqrt{\frac{72}{7}}\;\mu \tag{33}$$

Combining these two,

$$\left|\left\langle 7/2\|M^{(1)}\|7/2\right\rangle\right|^2 \; \left|\left\langle 1/2\|T^{(1)}\|3/2\right\rangle\right|^2 = \frac{4725}{32}\; a_{6p_{3/2}}^2 \tag{34}$$

Inserting this into Eq. (19), we find that only the $F = 3$ and 4 states are modified

$$W_3^{(2)} = \frac{675}{256}\; \frac{a_{6p_{3/2}}^2}{\Delta} \tag{35}$$

$$W_4^{(2)} = \frac{875}{256}\; \frac{a_{6p_{3/2}}^2}{\Delta}, \tag{36}$$

$$\begin{aligned} \Delta &= E_{6p_{3/2}} - E_{6p_{1/2}} \\ &= 554.11 \text{ cm}^{-1} \\ &= 1.6611 \times 10^7 \text{ MHz} \end{aligned}$$

It may be more accurate to replace

$$a_{6p_{3/2}}^2 \rightarrow \frac{1}{5}\; a_{6p_{1/2}} a_{6p_{3/2}}$$

since $\langle 6p_{1/2}\|T^{(1)}\|6p_{3/2}\rangle$ has contributions from both states. With this replacement, we find

$$W_3^{(2)} = \frac{135}{256}\; \frac{a_{6p_{1/2}} a_{6p_{3/2}}}{\Delta} \tag{37}$$

$$W_4^{(2)} = \frac{175}{256}\; \frac{a_{6p_{1/2}} a_{6p_{3/2}}}{\Delta}, \tag{38}$$

The relative size of the second-order energy is governed by the ratio

$$\rho_{1/2} = \frac{a_{6p_{1/2}}}{\Delta} = 1.757 \times 10^{-5}.$$

Thus, we may write

$$W_3^{(2)} = \frac{135}{256}\; \rho_{1/2}\; a_{6p_{3/2}} \tag{39}$$

$$W_4^{(2)} = \frac{175}{256}\; \rho_{1/2}\; a_{6p_{3/2}}, \tag{40}$$

1.4 Phenomenology for the $6p_{3/2}$ state

Let us temporarily ignore the second-order correction. For the $I = 7/2$, $J = 3/2$ level of Cs, we have from Eq. (17)

$$W_2^{(1)} = -\frac{27}{4}\, a + \frac{15}{28}\, b - \frac{33}{7}\, c \tag{41}$$

$$W_3^{(1)} = -\frac{15}{4}\, a - \frac{5}{28}\, b + \frac{55}{7}\, c \tag{42}$$

$$W_4^{(1)} = \frac{1}{4}\, a - \frac{13}{28}\, b - \frac{33}{7}\, c \tag{43}$$

$$W_5^{(1)} = \frac{21}{4}\, a + \frac{1}{4}\, b + c \tag{44}$$

The levels W_F are not independent. They satisfy the sum rule

$$\sum_F (2F+1) W_F^{(1)} = 0. \tag{45}$$

If we define $\Delta W_F = W_F^{(1)} - W_{F-1}^{(1)}$, then we find

$$\Delta W_3 = 3\,a - \frac{5}{7}\,b + \frac{88}{7}\,c \tag{46}$$

$$\Delta W_4 = 4\,a - \frac{2}{7}\,b - \frac{88}{7}\,c \tag{47}$$

$$\Delta W_5 = 5\,a + \frac{5}{7}\,b + \frac{40}{7}\,c \tag{48}$$

This set is independent and can be solved for $\{a,\, b,\, c\}$.

$$a = \frac{11}{120}\,\Delta W_5 + \frac{2}{21}\,\Delta W_4 + \frac{3}{56}\,\Delta W_3 \tag{49}$$

$$b = \frac{77}{120}\,\Delta W_5 - \frac{1}{3}\,\Delta W_4 - \frac{5}{8}\,\Delta W_3 \tag{50}$$

$$c = \frac{7}{480}\,\Delta W_5 - \frac{1}{24}\,\Delta W_4 + \frac{1}{32}\,\Delta W_3 \tag{51}$$

We use the data (given in MHz units) from Tanner and Wieman [2]

$$\Delta W_5 = 251.00(2) \tag{52}$$

$$\Delta W_4 = 201.24(2) \tag{53}$$

$$\Delta W_3 = 151.21(2) \tag{54}$$

and solve for $\{a,\, b,\, c\}$ to obtain

$$a = 50.2746 \pm 0.0028 \tag{55}$$

$$b = -0.5279 \pm 0.0191 \tag{56}$$

$$c = 0.00073 \pm 0.00108 \tag{57}$$

These values are consistent with the values found in Ref.[2]:

$$a = 50.275(3) \tag{58}$$

$$b = -0.53(2) \tag{59}$$

An improvement in precision by a factor ten would provide evidence for a nuclear octupole moment! Indeed, Gerginov et al. [3] obtained $c = 0.56(7)$ kHz from their measurements of the hyperfine intervals. From their measurements, they inferred $Q = -3.22(4)$ mb for the nuclear quadrupole moment and $\Omega = 0.82(10)$ bμ_N. With the data from [3], we write

$$\Delta W_5 = 251.0916(20) \tag{60}$$

$$\Delta W_4 = 201.2871(11) \tag{61}$$

$$\Delta W_3 = 151.2247(16). \tag{62}$$

We obtain

$$a = 50.28827(23) \quad (63)$$
$$b = -0.4934(17) \quad (64)$$
$$c = 0.00056(7) \quad (65)$$

using the 2nd-order analysis given in the following subsection. These values agree precisely with those obtained in [3].

1.5 Analysis including 2nd-order perturbation

Let us include the second-order corrections. We let $W_F = W_F^{(1)} + W_F^{(2)}$ and find

$$W_2 = -\frac{27}{4}\,a - \frac{15}{28}\,b - \frac{33}{7}\,c \quad (66)$$
$$W_3 = -\left[\frac{15}{4} - \frac{135}{256}\,\rho_{1/2}\right]a - \frac{5}{28}\,b + \frac{55}{7}\,c \quad (67)$$
$$W_4 = \left[\frac{1}{4} + \frac{175}{256}\,\rho_{1/2}\right]a - \frac{13}{28}\,b - \frac{33}{7}\,c \quad (68)$$
$$W_5 = \frac{21}{4}\,a + \frac{1}{4}\,b + c \quad (69)$$

These equations can be solved for $\{a, b, c\}$. They appear to be relevant only for the precise measurements in [3].

Thanks are owed to K. Calkins for suggestions on this manuscript.

References

[1] I. Lindgren and J. Morrison, *Atomic Many-Body Theory* (Springer Verlag, Berlin, 1986), 2nd ed.

[2] C. E. Tanner and C. E. Wieman, Phys. Rev. A **38**, 1616 (1988).

[3] V. Gerginov, A. Derevianko, and C. E. Tanner, Phys. Rev. Lett **91**, 072501 (2003).