Off-diagonal hyperfine interaction between the $6p_{1/2}$ and $6p_{3/2}$ levels in $^{133}$Cs

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The off-diagonal hyperfine interaction between the $6p_{1/2}$ and $6p_{3/2}$ states in $^{133}$Cs is evaluated in third-order MBPT giving 37.3 and 48.3 Hz, respectively, for second-order energies of the $6p_{3/2}$ $F = 3$ and $F = 4$ levels. This result is a factor of 10 smaller than one obtained from an uncorrelated first-order Dirac–Hartree–Fock calculation and used in the analysis of a recent high-precision ($\approx 2$ kHz) measurement of the $6p_{3/2}$ hyperfine structure [Gerginov et al. Phys. Rev. Lett. 91, 72301 (2003)]. The factor of 10 difference has negligible effect on the conclusions of the recent experiment but will become important for experiments carried out at a precision of better than 1 kHz.

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I. INTRODUCTION

In the recent study of the hyperfine structure of the $6p_{3/2}$ state of $^{133}$Cs by Gerginov et al. [1], intervals between hyperfine levels were measured to an accuracy of $\approx 2$ kHz, which was sufficient to give, for the first time, a nonzero value for the $c$ hyperfine constant. The value of the nuclear octupole moment of $^{133}$Cs obtained from $c$ was $\Omega = 0.82(10) b \mu_N$, which is about a factor of 40 larger than nuclear shell-model prediction $\Omega_{\text{n.s.m.}} = 0.022 b \mu_N$, motivating a reexamination of corrections to the hyperfine constants. One such correction is the second-order hyperfine interaction between the $6p_{3/2}$ and $6p_{1/2}$ states. An estimate of this correction, based on an independent particle model of the cesium atom, was used in Ref. [1]. In the present work, we carry out a detailed third-order MBPT calculation and obtain corrections to the $6p_{3/2}$ hyperfine levels that are a factor of 10 smaller than the values used in Ref. [1]. Revised values of the hyperfine constants $a$, $b$, and $c$, obtained using the present results for the second-order hyperfine energies, agree with those reported in Ref. [1] to within the error estimates. However, for future experiments, especially experiments aimed at a precision of better than 1 kHz, it will be important to use the correlated values of the corrections presented here, rather than the larger values given in Ref. [1].

II. PERTURBATION EXPANSION

We write the hyperfine interaction in the form

$$H_{hf} = \sum_{k\lambda} (-1)^s T_{\lambda}(s) M^{(s)}_{\lambda}$$

where $T_{\lambda}(s)$ is an irreducible tensor operator acting in the electron sector and $M^{(s)}_{\lambda}$ is an irreducible tensor operator acting in the nuclear sector. The first-order hyperfine correction to the energy of a state $|1\rangle$ is

$$W^{(1)}_E = \langle 1|H_{hf}|1\rangle = \sum_k (-1)^{J_s+J_F+J} \left\langle J \mid s \rangle T^{(s)} \langle J \mid J_I \mid M^{(s)} \rangle \mid J \rangle.$$
\[ W_F^{(1)} = \frac{1}{2}K^a + \frac{3K^e + 4J^eJ^a}{8L(2I-1)J(2J-1)}b \]
\[ + \frac{5K^f (K + 4) - 4K[3J^eJ^a - J^e - J^a - 3] - 20J^eJ^a}{I(2I-1)(2J-2)(2J-1)(2J-2)}c, \]

where \( I_1 = I(I+1), \ J_1 = J(J+1), \ F_2 = F(F+1), \ K = F_2 - J_1 + I_1, \) and \( K_1 = K(K+1). \)

The second-order (in the hyperfine interaction) energy of a state is given by

\[ W_F^{(2)} = \sum_{n\neq 1} \frac{|\langle H_{ad}|n\rangle \langle n|H_{ad}|1\rangle|}{E_1 - E_n}. \]

For the state \(|1\rangle = |6p_{3/2}\rangle\) of Cs, the second-order hyperfine energy is dominated by the single state \(|2\rangle = |6p_{1/2}\rangle\). Moreover, the largest contribution from this state is the one associated with the magnetic dipole term \(k = k^d = 1\). After angular reduction, the second-order energy is

\[ W_F^{(2)} = \left\{ \begin{array}{l} J_1 \quad F \\ J_1 \quad J_1 \quad 1 \end{array} \right\} \frac{2|\langle J_1|T(1)|I_1\rangle|^2|\langle J_1|M(1)|I\rangle|^2}{E_1 - E_2}. \]

The contributions to the second-order energy from the nuclear quadrupole moment have been evaluated in lowest order and found to change the values obtained from Eq. (5) by less than 1%. The fine-structure interval \(E_1 - E_2\) in the denominator is determined as the difference between \(f_{d2}\) the centroid of the \(6s^23p_{1/2} \rightarrow 6p^2P_{3/2}\) transition [2,3] and \(f_{d1}\) the centroid of the \(6s^23p_{1/2} \rightarrow 6p^2P_{1/2}\) transition [4], both of which have been measured to high precision. One obtains \(E_1 - E_2 = f_{d2} - f_{d1} = 1.666 \times 10^7 \text{ MHz}\).

\[ W_F^{(2)} = 1.660 \times 10^7 \text{ MHz}. \]

\[ w_{3/2} = 1.5 \times 10^7 \text{ MHz}. \]

\[ W_3 - W_4 = 251.0916 \pm 0.0617 \text{ MHz}. \]

\[ W_4 - W_3 = 251.0916 \pm 0.0617 \text{ MHz}. \]

\[ W_3 - W_2 = 151.2247(16) \text{ MHz}. \]

\[ W_2 - W_1 = 251.0916 \pm 0.0617 \text{ MHz}. \]

\[ W_1 - W_0 = 251.0916 \pm 0.0617 \text{ MHz}. \]

The estimates made in the previous section depend on the assumption that correlation corrections to reduced matrix elements of the hyperfine operator \(|\langle T^{(1)}|j\rangle|\) are independent of the total angular momentum \(J\) of the \(6p\) state. To test that assumption, we carried out correlations third-order MBPT calculations of the \(6p\) matrix elements.

In Table I, we give a detailed breakdown of contributions to the third-order matrix elements. Formulas for the first-, second-, and third-order matrix elements are given in Ref. [5]. We use a modified version of these formulas in which \(a\) the sum of the second-order matrix element and \(b\) the third-order contribution to the random-phase approximation (RPA) is replaced by the exact solution of the EPA equations, and \(b\) all one-electron matrix elements in third-order are replaced by their EPA counterparts. These modifications give dipole transition matrix elements that are gauge invariant in second- and third-order [6]. The third-order hyperfine constants for the \(6p_{3/2}\) and \(6p_{1/2}\) states evaluated in this way are within a few percent of experiment. Since we use the same method to evaluate diagonal and off-diagonal matrix elements, we expect the third-order off-diagonal matrix element to be accurate to a few percent.

Substituting the third-order off-diagonal matrix element given in Table I into Eq. (5), we find \(W_3^{(2)} = 37.3 \text{ Hz}\) and \(W_4^{(2)} = 48.3 \text{ Hz}\) for the \(6p_{3/2}\) state. Combining the second-order corrections with the observed \(6p_{3/2}\) hyperfine intervals (MHz) from [1].

\[ W_3 - W_4 = 251.0916(20), \]
\[ W_4 - W_3 = 201.2871(11), \]
\[ W_3 - W_2 = 151.2247(16), \]
we obtain the following values for the hyperfine constants (MHz):

\[ a = 50.288\,25(23), \]
\[ b = -0.4940(17), \]
\[ c = 0.000\,56(7). \]

These values agree within error limits with those found in Ref. [1].

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