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 ($\leqslant$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 $\leqslant$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 $\Omega_{\text{n.s.m.}} = 0.022b\ \mu_N$, 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

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

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. The first-order hyperfine correction to the energy of a state $|1\rangle$ is

$$W^{(1)}_F = \langle 1|H_{\text{hf}}|1\rangle = \sum_k (-1)^{I+J+F} \begin{Bmatrix} J & I & F \\ I & J & k \end{Bmatrix} \langle J\|T^{(k)}\|J\rangle \langle I\|M^{(k)}\|I\rangle.$$

The nuclear matrix elements are given in terms of conventional nuclear moments through

$$\langle II|M^{(1)}_0|II\rangle = \mu,$$

$$\langle II|M^{(2)}_0|II\rangle = \tfrac{1}{2}Q,$$

$$\langle II|M^{(3)}_0|II\rangle = -\Omega.$$

Here, μ is the nuclear magnetic dipole moment, *Q* is the nuclear electric quadrupole moment, and Ω is the nuclear magnetic octupole moment. With these definitions, we introduce the conventional hyperfine constants *a*, *b*, and *c* through the relations

$$a = \frac{\mu}{IJ}\langle JJ|T^{(1)}_0|JJ\rangle, \tag{1}$$

$$b = 2Q\langle JJ|T^{(2)}_0|JJ\rangle, \tag{2}$$

$$c = -\Omega\langle JJ|T^{(3)}_0|JJ\rangle, \tag{3}$$

and write the first-order hyperfine energy as

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$$W_F^{(1)} = \frac{1}{2}Ka + \frac{3K_+ - 4J_+I_+}{8I(2I-1)J(2J-1)}b + \frac{5K^2(K+4) - 4K[3J_+I_+ - J_+ - I_+ - 3] - 20J_+I_+}{I(2I-1)(2I-2)J(2J-1)(2J-2)}c, \quad (4)$$

where $I_+ = I(I+1)$, $J_+ = J(J+1)$, $F_+ = F(F+1)$, $K = F_+ - J_+ - I_+$, and $K_+ = K(K+1)$.

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

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

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

$$W_F^{(2)} = \begin{Bmatrix} J_2 & I & F \\ I & J_1 & 1 \end{Bmatrix}^2 \frac{|\langle J_2\|T^{(1)}\|J_1\rangle|^2 |\langle I\|M^{(1)}\|I\rangle|^2}{E_1 - E_2}. \quad (5)$$

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 $6s^2S_{1/2} \rightarrow 6p^2P_{3/2}$ transition [2,3] and f_{D1} the centroid of the $6s^2S_{1/2} \rightarrow 6p^2P_{1/2}$ transition [4], both of which have been measured to high precision. One obtains $E_1 - E_2 = f_{D2} - f_{D1} = 1.660\,966\,966\,7(11) \times 10^7$ MHz.

III. NUMERICAL ESTIMATES

Correlation corrections to hyperfine matrix elements in alkali-metal atoms are large. Thus, for example, a lowest-order Dirac–Hartree–Fock calculation of the hyperfine constant $a_{3/2}$ for the $6p_{3/2}$ state of Cs (which is proportional to the diagonal matrix element $\langle 3/2\|T^{(1)}\|3/2\rangle$) leads to a result that is a factor of 2 smaller than the experimental value. One expects (and indeed finds) corrections of a similar size for the off-diagonal matrix element $\langle 1/2\|T^{(1)}\|3/2\rangle$ appearing in the numerator of the expression for the second-order hyperfine energy. If we assume that the relative size of the correlation corrections to the two matrix elements mentioned above are the same, then we can determine the ratio $\langle 1/2\|T^{(1)}\|3/2\rangle / \langle 3/2\|T^{(1)}\|3/2\rangle$ by means of a lowest-order calculation and, using that ratio together with the experimental value of $a_{3/2}$, obtain an accurate value for $\langle 1/2\|T^{(1)}\|3/2\rangle$. That was the strategy used to obtain the values $W_3^{(2)} = 401$ Hz and $W_4^{(2)} = 520$ Hz for the $6p_{3/2}$ state of ^{133}Cs quoted in Ref. [1]. (The ratio of matrix elements was determined in the nonrelativistic approximation and did not depend on details of the $6p$ wave function. The nonrelativistic approximation is not a serious problem, however, since the ratio obtained using relativistic Dirac–Hartree–Fock wave functions differs from the nonrelativistic ratio by less than 5%.)

TABLE I. MBPT contributions to the hyperfine constants $a_{1/2}$ and $a_{3/2}$ (MHz) of the $6p_{1/2}$ and $6p_{3/2}$ states, respectively, and to the off-diagonal matrix element $gT^{(1)} = g_I\langle 1/2\|T^{(1)}\|3/2\rangle$(MHz) are presented. The resulting third-order hyperfine constants are are compared with experiment.

Term	$a_{1/2}$	$a_{3/2}$	$gT^{(1)}$
1st	160.88	23.92	26.97
2nd	40.66	18.84	−34.15
Bruck[a]	84.40	16.08	−1.12
St Rad[a]	5.43	−7.51	24.85
Norm	−1.20	−0.23	0.04
3rd	88.62	8.33	23.77
Total	290.17	51.09	16.59
Expt.	291.89	50.29	

[a]Third-order Brueckner orbital and structural radiation corrections, as defined in Ref. [5].

IV. CORRELATION CORRECTIONS

The estimates made in the previous section depend on the the assumption that correlation corrections to reduced matrix elements of the hyperfine operator $\langle j\|T^{(1)}\|j'\rangle$ are independent of the total angular momentum j of the $6p_j$ state. To test that assumption, we carried out correlated third-order MBPT calculations of the three $6p_j$ 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 element 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 the third-order contribution to the random-phase approximation (RPA) is replaced by the exact solution to the RPA equations, and (b) all one-electron matrix elements in third-order are replaced by their RPA 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 $6p_{1/2}$ and $6p_{3/2}$ 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 $W_3^{(2)} = 37.3$ Hz and $W_4^{(2)} = 48.3$ Hz for the $6p_{3/2}$ state. Combining the second-order corrections with the observed $6p_{3/2}$ hyperfine intervals (MHz) from [1],

$$W_5 - W_4 = 251.0916(20),$$

$$W_4 - W_3 = 201.2871(11),$$

$$W_3 - W_2 = 151.2247(16),$$

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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