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Calculation of A and B hyperfine structure factors for 31 levels of Cs II

Jorge Mahecha G.

Departamento de Física, Universidad de Antioquia. Apdo. Aéreo 1226, Medellín, Colombia

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Abstract. Theoretical values of hyperfine structure constants of Cs II for magnetic dipole moment interaction (A) and electric quadrupole moment interaction (B) are calculated using the effective operator method proposed by Sandars and Beck and developed by Childs and Goodman. Reported A values are compared with some known experimental results. Calculations were made using a computer program applicable to any atom or ion whose external electrons have configuration $l^N l'$.

Resumen. Se calculan valores teóricos de las constantes de estructura hiperfina de Cs II para la interacción dipolar magnética (A) y la interacción cuadrupolar eléctrica (B) usando el método de los operadores efectivos propuesto por Sandars y Beck y desarrollado por Childs y Goodman. Los resultados obtenidos para A se comparan con algunos valores experimentales disponibles. Los cálculos fueron hechos con ayuda de un programa de computador aplicable a cualquier átomo o ion cuyos electrones externos posean la configuración $l^N l'$.

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1. Introduction

The use of tunable lasers has given a very great advance in the studies of hyperfine structure (HFS) in free atoms and ions.

The first HFS quantum-mechanical studies were made on one-electron atoms. In the early 40's, Racah developed elegant methods to calculate matrix elements of tensor operators between atomic

states (multiplets), in the atomic shell model [1]. It was only in 1953 that methods were applied to the HFS of many-electron atoms by Trees, who obtained very good results for the ^{55}Mn [2]. In 1955 Schwartz combined the Racah methods with Dirac's equation to study HSF in one-electron atoms [3]. In 1965, Sandars and Beck obtained a theory of HFS of complex atoms using the effective operator formalism [4]. On the basis of that theory, Childs and Goodman found a formula for the HFS constants A and B of the states of a $l^N l'$ configuration is LS coupling, and obtained results well fitted with the experiments [5, 6].

The first observations of HFS were based on high resolution optic spectroscopy in beam experiments [21], but the advances were faster with the introduction of the radiofrequency spectroscopy in atomic beams, following Rabi and others [21]. With those methods, accurate values of the hyperfine factors of the ground state and first excited states of atoms were obtained. In 1950 Kastler [33] discovered the optical pumping techniques, which greatly facilitate the measurements of HFS constants of excited states with laser spectroscopy techniques.

The theories of HFS provide sensitive tests of the effects of superposition of configurations, as we will have opportunity to show in this work.

The Cs II ion is a member of the isoelectronic sequence of Xe I and its energy level structure is similar to that of a rare gas. The ground state is $5p^6\,{}^1S_0$ and the configurations that give the first eleven excited states are $5p^5 5d$ and $5p^5 6s$. Five levels of those configurations have $J = 1$; this is why they have transitions to the ground state. The six levels with $J > 1$ are metastable and some of them can be used to populate the upper levels $5p^5 6p$ with laser pumping.

In 1931 Kopferman made the first measurements of the HFS of Cs II and deduced that the value of the nuclear spin of ^{133}Cs is 7/2 [7]. Reader in 1976 analyzed the current information and made a new classification of the levels of Cs II based on a different coupling than LS [11]. Alvarez *et al.* measured the HFS intervals of Cs II with the interaction of a ion beam with laser radiation, and obtained the

constants of magnetic dipole interaction with good precision, and with less precision the electric quadrupole interaction constants [8].

In this work, the main results of the theory of hyperfine structure of complex atoms are reviewed first. Then, a sketch of the procedure to calculate A and B as sums of terms, each formed with a factor coming from angular moment considerations and a radial factor, is given. Then, the angular and radial coefficients are calculated, and with them the values of A and B are obtained. Regarding A, it is in good agreement with experiments only in the levels without strong configuration mixing, but as a result of this calculation we can estimate the configuration mixing effects on the values of the HFS constants A. Our results for Cs II are analogous to results reported by Childs for ^{51}V [32]. Values of B are also reported, but there are not experimental results for comparison. Some improvement of A values had been obtained with a least square fit to experimental values.

2. The energy levels for Cs II

Reader [11], found that Cs II energy levels are properly described by using a coupling scheme of the kind $J_1 l$. The notation for that coupling is nl, $n'l'\, J_1[K]_J$, where nl are quantum numbers of external core electrons, $n'l'$ are quantum numbers of excited electron and the quantum numbers of the core states in LS coupling are L_1, S_1, J_1 [9, 10].

Figure 1 shows the relative disposition of the first excited levels, and some optically allowed transitions among them. Because of the hyperfine interaction, the levels $5d[7/2]^{\circ}_4$, $5d[3/2]^{\circ}_2$, $6p[5/2]_3$ and $6p[3/2]_1$ are split in 8, 5, 7 and 3 sublevels since nuclear spin of ^{133}Cs is 7/2.

Reader also found the percentual composition of the states of the configurations $5p^5(5d + 6s)$ and $5p^5 6p$, with $J_1 l$ coupling. He found significant superposition of configurations. Reader obtained his results by diagonalizing the energy matrix in states built with Hartree-Fock wave functions and different types of coupling. The

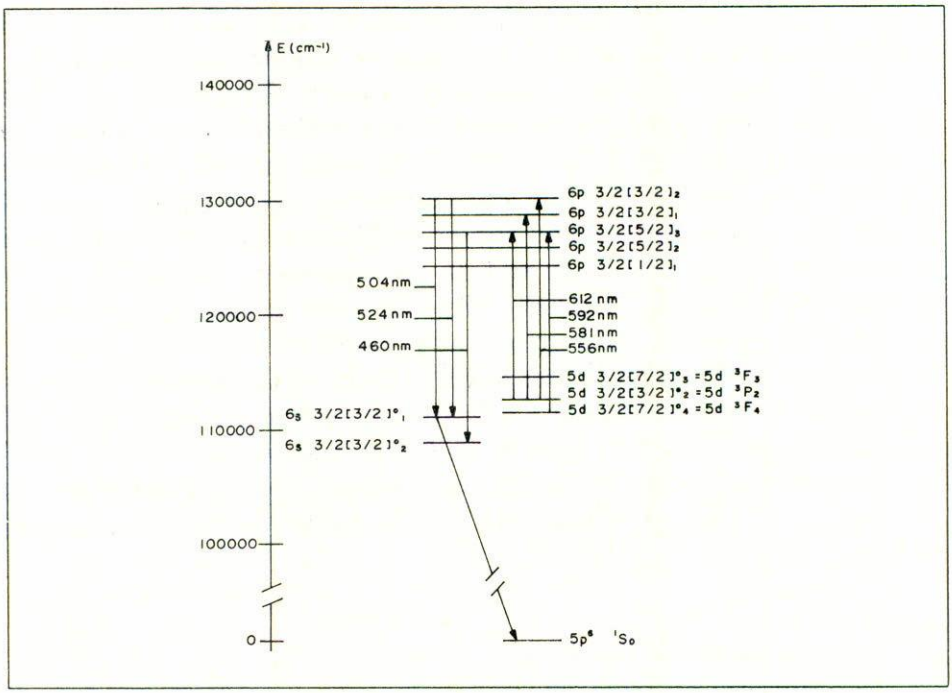

FIGURE 1. Partial diagram of the energy levels of Cs II [30].

states with the best fits to experimental results are shown in his tables.

3. The hyperfine hamiltonian

This Hamiltonian describes the perturbation on the fine structure levels produced by the interaction among the atomic relativistic electrons and charges and currents in the nucleus not included in the unperturbed Hamiltonian. That perturbation is

$$H_{\text{h.f.}} = \sum_{i=1}^{N} \left[\frac{Ze^2}{r_i} - eV(\mathbf{r}_i) + e\boldsymbol{\alpha}_i \cdot \mathbf{A}(\mathbf{r}_i) \right], \tag{1}$$

where $\mathbf{r}_i$ is the vector position of the i-th electron, $\mathbf{A}$ and V the vector and scalar potentials due to the nucleus and $\boldsymbol{\alpha}$ is a Dirac matrix.

Now, the potentials V and $\mathbf{A}$ can be written as multipole expansions, that is, as products of tensor operators corresponding to electrons and nucleus. The calculation was made by Schwartz [3], with the result,

$$H_{\text{h.f.}} = \sum_{i=1}^{N} \sum_{k>0} \left\{ \frac{-e}{r_i^{k+1}} \mathbf{C}_i^{(k)} \cdot \mathbf{F}^{(k)} + \frac{ie}{r_i^{k+1}} \left[\frac{k+1}{k} \right]^{1/2} (\boldsymbol{\alpha}_i \mathbf{C}_i^{(k)})^{(k)} \cdot \mathbf{N}^{(k)} \right\}. \tag{2}$$

$C_{qi}^{(k)}$ is proportional to the spherical harmonic $Y_{kq}(\theta_i, \phi_i)$ of the i-th electron. $F_q^{(k)}$ is the electrostatic nuclear operator composed of a sum of terms, each proportional to a spherical harmonic of a nucleon. $N_q^{(k)}$ is the magnetic nuclear operator composed of contributions of orbital angular momentum and spin of each nucleon. Details can be seen in Armstrong's book, Ch. IV [13].

$\mathrm{H}_{\text{h.f.}}$ contains only one-electron operators.

$$H_{\text{h.f.}} = \sum_{i=1}^{N} \sum_{k=1}^{\infty} \left[\mathbf{Q}^{(k)}(r_i) \cdot \mathbf{F}_n^{(k)} + \mathbf{M}^{(k)}(r_i) \cdot \mathbf{N}_n^{(k)} \right]. \tag{3}$$

The subscripts i and n denote electron and nuclear operators respectively. $k = 1$ describes the electric dipole interaction and $k = 2$ the magnetic quadrupole interaction; those values of k give the main contributions in (3). For $k = 1$ only the M-term contributes and for $k = 2$, the Q-term. $\mathbf{F}$ and $\mathbf{N}$ are tensor operators describing the nuclear magnetic and electric moments. The second quantization representation of this operator contains matrix elements of the form $(nljm|\mathbf{T}^{(k)}(r)|n'l'j'm')$ multiplied by creation and annihilation operators of one-electron states, $q^{\dagger}(nljm)q(n'j'l'm')$.

Then, the electronic part of this operator can be written in second quantization in the form [13]

$$H_{\text{h.f.}} = \sum_{k=1}^{\infty} \left[\mathbf{Q}^{(k)} \cdot \mathbf{F}_n^{(k)} + \mathbf{M}^{(k)} \cdot \mathbf{N}_n^{(k)} \right]. \tag{4}$$

This operator is adapted to calculate the HFS energy if one knows the full atomic relativistic states. As is well known, the relativistic calculations must be carried in the jj coupling scheme. However, one usually knows the wave functions as expansions in functions with LS coupling. It is desirable to use the relativistic operator (4) in a nonrelativistic way. That goal was achieved by Sandars and Beck [4].

They introduced an effective HFS operator defined by the relation

$$\langle nljm | H_{\text{h.f.}}^{\text{eff.}} | n'l'j'm' \rangle = (nljm | H_{\text{h.f.}} | n'l'j'm'), \tag{5}$$

where the states $|nljm\rangle$ are the nonrelativistic limits of the Dirac states $|nljm\rangle$, and $H_{\text{h.f.}}$ is the operator [4]

$$H_{\text{h.f.}}^{\text{eff.}} = \sum_{k=1}^{\infty} \mathbf{T}_e^{(k)\text{eff.}} \cdot \mathbf{T}_n^{(k)}. \tag{6}$$

The tensor operators $\mathbf{T}_e^{(k)\text{eff.}}$ can be expanded in a basis $\mathbf{U}^{(k_l k_s)k}$ for the k-order tensors obtained by coupling orbital and spin tensor operators [4],

$$\mathbf{T}_e^{(k)\text{eff.}} = \sum_{k_l} \sum_{k_s} P^{(k_l k_s)k} \mathbf{U}^{(k_l k_s)k}. \tag{7}$$

Now, replacing (6) and (7) in (5), and after some Racah algebra one can express the numbers $P^{(k_l k_s)k}$ as combination of reduced matrix elements of $\mathbf{T}_e^{(k)}$, in the relativistic states, $(nlj \| \mathbf{T}_e^{(k)} \| n'l'j')$. That is the technique of the effective operator developed by Sandars and Beck.

4. The effective HFS hamiltonian for configurations $l^N l'$

The effective HFS Hamiltonian has the form,

$$H_{\text{h.f.}} = \sum_{k=1}^{\infty} \left[\mathbf{Q}_e^{(k)\text{eff.}} \cdot \mathbf{F}_n^{(k)} + \mathbf{M}_e^{(k)\text{eff.}} \cdot \mathbf{N}_n^{(k)} \right]. \tag{8}$$

$\mathbf{Q}_e^{(k)\text{eff.}}$ and $\mathbf{M}_e^{(k)\text{eff.}}$ have an expansion as in (7). The result [4, 13] shows that $\mathbf{Q}^{(2)}$ and $\mathbf{M}^{(1)}$ depend linearly on some radial parameters $a_l^{k_l k_s}$ and $b_l^{k_l k_s}$ respectively. They are combinations of some radial integrals, which depend on the relativistic radial functions, in principle derivable by using relativistic Hartree-Fock methods. Casimir [17] obtained approximate expressions for those integrals in a many-electron atom expressed in terms of an effective charge and some relativistic correction factors. With this approximation, the relativistic radial integrals are proportional to the nonrelativistic ones. Kopferman [7] presents tables and formulas of the Casimir's relativistic factors. See details in the Armstrong's book, Ch. VIII [13].

The expression for the magnetic dipole part of the effective HFS Hamiltonian is

$$H_{\text{h.f.}}(M1) = \left\{ \sum_{i=1}^{N} \left[a_l^{01} \mathbf{l}_i - 10^{1/2} a_l^{12} (\mathbf{s}\, \mathbf{C}^{(2)})_i^{(1)} + a_l^{10} \mathbf{s}_i \right] \right. \tag{9}$$
$$\left. + \left[a_l^{01} \mathbf{l}_{N+1} - 10^{1/2} a_l^{12} (\mathbf{s}\, \mathbf{C}^{(2)})_{N+1}^{(1)} + a_l^{10} \mathbf{s}_{N+1} \right] \right\} \cdot \mathbf{I},$$

and represents the interaction between the magnetic moments of electrons and nucleus.

The expression for the electric quadrupole part of the effective HFS Hamiltonian is

$$
\begin{aligned}
H_{\text{h.f.}}(E2) = \frac{r_n^2}{Q}\,\mathbf{C}_n^{(2)} \cdot \sum_{i=1}^{N} \Big[& b_l^{02}\mathbf{C}_i^{(2)} + (3/10)^{1/2} b_l^{11} (\mathbf{s}_i \mathbf{l}_i)^{(2)} \\
& + (3/10)^{1/2} b_l^{13} (\mathbf{s}_i (\mathbf{C}_i^{(4)} \mathbf{l}_i)^{(3)})^{(2)} \Big] \\
& + \frac{r_n^2}{Q}\mathbf{C}_n^{(2)} \cdot \Big[b_l^{02}\mathbf{C}_{N+1}^{(2)} + (3/10)^{1/2} b_l^{11} (\mathbf{s}_{N+1} \mathbf{l}_{N+1})^{(2)} \\
& + (3/10)^{1/2} b_l^{13} (\mathbf{s}_{N+1} (\mathbf{C}_{N+1}^{(4)} \mathbf{l}_{N+1})^{(3)})^{(2)} \Big],
\end{aligned}
\tag{10}
$$

where Q is the nuclear quadrupole moment, and a_l^{LS} and b_l^{LS} are linear combinations of Casimir factors, and are proportional respectively to a_{nl} and b_{nl}, defined by Childs [5]. This Hamiltonian represents the interaction between the electric quadrupole moments of nucleus and electrons.

5. Matrix elements of $H_{\text{h.f.}}^{\text{eff.}}$

The non-relativistic atomic states of a configuration $l^N l'$ in LS coupling are $|l^N \alpha_1 L_1 S_1, s'l'; SLJIFM\rangle$ where $\alpha_1 L_1 S_1)$ are the quantum numbers of the core, and $s'l'$ are quantum numbers of the external electron. Reader's tables [11] give the expansion coefficients for the $J_1 l$ states in terms of the LS states. For example, $5p^5 6p\, 1/2[3/2]_1 = -46\%^3 D_1 - 34\%^1 D_1 + 20\%^3 P_1$. Reader found that some energy levels can have contributions from several configurations.

In the calculation of the matrix element, for example of the $\sum \mathbf{l}_i$-term in (9), one uses the Wigner-Eckart theorem; then a 3-j coefficient appears and a reduced matrix element in the coupled states $|JIF\rangle$. In expressing that reduced matrix element we get a 6-j coefficient and other reduced matrix element in the coupled states $|LSJ\rangle$. Now we solve for the reduced matrix element only

between the core states and get a new 6-j coefficient; finally, we express the reduced matrix element in the orbital states of the core and get another 6-j coefficient. In those terms of (9) containing tensor products of spin and orbital operators, the reduced matrix elements in the core states break out in a product of orbital and spin reduced matrix elements, with 9-j coefficients; in the orbital factor the reduced matrix element of a Racah's orbital unit tensor operator appears [27].

Childs [6] applies the mentioned procedure to calculate the non-diagonal matrix elements of $H^{\text{eff.}}_{\text{h.f.}}$. The final result for the magnetic dipole term have the form,

$$\begin{aligned}\langle l^N \alpha_1 L_1 S_1, s'l'; LSJIFM | H^{\text{eff.}}_{\text{h.f.}} | l^N \alpha'_1 L'_1 S'_1, s'l'; L'S'J'IFN\rangle \\ = \Gamma_1(JJ'IF)[P_1(P_2 a_l^{01} + P_3 a_l^{01}) + P_4(P_5 a_l^{12} + P_6 a_l^{12}) \\ + P_7(P_8 a_l^{10} + P_9 a_l^{10})].\end{aligned} \tag{11}$$

The factor Γ_1 comes from uncoupling the nuclear and electronic parts, and is defined by,

$$\begin{aligned}\Gamma_1(JJ'IF) = (-1)^{J'+I+F}[I(I+1)(2I+1)(2J+1)(2J'+1)]^{1/2} \\ \times \begin{Bmatrix} J & J' & 1 \\ I & I & F \end{Bmatrix}.\end{aligned} \tag{12}$$

In Eq. (11), the factor in front of Γ_1 represents the constant of hyperfine coupling A,

$$\langle FM | H^{\text{eff.}}_{\text{h.f.}}(M1) | FM\rangle = A\langle FM | \mathbf{I}\cdot\mathbf{J} | FM\rangle. \tag{13}$$

A is a characteristic constant of the non splitted level, that is, dependent only on L, S, J and I but not on the total angular moment F of the coupled system of electrons and nucleons. It characterizes the HFS splitting.

The coefficients $P_1, \ldots, P_9$ have long expressions in terms of the 6-j and 9-j coefficients, and P_5 depends also on the reduced matrix elements of the Racah's unit tensor $\mathbf{V}^{(12)}$ between states of the core.

The nondiagonal matrix elements of the electric quadrupole interaction term is analogous to (11), with another factor Γ_2, with b_1^{LS} in the place of a_l^{LS}, and $P_1, \ldots, P_9$ replaced by $Q_1, \ldots, Q_9$. Now Q_2, Q_5 and Q_8 depend on the reduced matrix elements of the Racah's unit tensors $\mathbf{U}^{(2)}$, $\mathbf{V}^{(13)}$, $\mathbf{V}^{(11)}$ respectively [5, 6].

$\Gamma_2(JJ'IF)$ is defined by an expression something similar to (12) containing in the $6j$-coefficient a 2 in the place of 1 [6], and the constant of hyperfine structure constant for electric quadrupole moment interaction B is defined by

$$\langle FM|H_{\mathrm{h.f.}}^{\mathrm{eff.}}(E2)|FM\rangle = B\Gamma_2(JJ'JF). \tag{14}$$

Constant A is proportional to nuclear gyromagnetic ratio μ_I/I and B is proportional to nuclear quadrupole moment Q_I.

In the calculations using Child's formulas it is necessary to evaluate the 6-j and 9-j coefficients by using standard formulas given in textbooks [27]. The reduced matrix elements of the operators $\mathbf{W}^{(\mathrm{LS})}$, proportional to Racah's tensors $\mathbf{U}$ and $\mathbf{V}$, can be calculated with a formula given by Judd [9, 15]. That formula depends on the fractional parentage coefficients, tabulated by Nielson and Koster [28] for the states of the configurations p^N, d^N and f^N, and on the states of the parent configuration l^{N-1}.

6. Numerical results

To compute the reduced matrix elements of the operators $\mathbf{V}^{(k_l k_s)}$, we notice that configuration p^5 has only one multiplet, with $S_1 = 1/2$ and $L_1 = 1$. Then the Judd's formula gives, $V^{(12)} = 1.2247448$, $U^{(2)} = -1$, $V^{(11)} = 1.2247448$, $V^{(13)} = 0$, for the elements $\langle p^5, {}^2P \|V^{(k_l k_s)}\| P^5, {}^2P\rangle$.

The parameters a_{nl} and b_{nl}, when $l \neq 0$, can be calculated from the fine structure constants ξ_{nl} for Cs II, found by Reader [11] using

a fitting to experimental results, with the formulas [2]

$$a_{nl} = \frac{0.545\xi_{nl}g(I) \times 10^{-3}}{H_r(l, Z_{\text{eff.}})Z_{\text{eff.}}},$$
$$b_{nl} = \frac{0.253\xi_{nl}Q \times 10^{21}}{H_r(l, Z_{\text{eff.}})Z_{\text{eff.}}I(2I-1)} \tag{15}$$

where ξ_{nl}, a_{nl}, b_{nl} are in Kaisers (cm^{-1}). H_r is a Casimir factor, and $g(I) = \mu_I/I$ is the nuclear gyromagnetic ratio. $\mu_I = 2.574$ nuclear magnetons and $I = 7/2$, for ^{133}Cs [29], so that, $g(I) = 0.735\mu_N$. Q is the nuclear quadrupole moment, with value $Q = -0.0033$ barn [29]. The results for a_{nl} and b_{nl} calculated with formulas (15) are shown in Table I.

nl	$5p$	$5d$	$6p$	$6d$
a_{nl}	2011.42	84.7145	233.4	19.226
b_{nl}	−0.1752	−0.00763	−0.021	−0.001653

TABLE I. Values of the parameters a_{nl}, b_{nl}, in Mhz obtained from a fit to spectroscopic results.

We have calculated the coefficients a_{ns}^{10} by using the following formula [9], coming from the contact terms of the HFS interaction [18, 19, 20]:

$$a_s^{10} = \frac{16\pi}{3}\mu_0\frac{\mu_I}{I}|\Phi_{ns}(0)|^2 F_r(1/2, Z_{\text{eff.}}). \tag{16}$$

$H_r(l, Z_{\text{eff.}})$ and $F_r(j, Z_{\text{eff.}})$ are Casimir relativistic factors [9] and Φ_{ns} is a one-electron nonrelativistic wave function.

We also notice that $a_s^{01} = a_s^{12} = 0$. To use (16) it is first necessary to know the value of the non-relativistic wave function at the position of the nucleus. We have numerically integrated the Schrödinger equation [23, 24, 25] with an analytical local selfconsistent potential [22], using the appropriate parameters for Cs II. Some error is

$n's$	$5s$	$6s$	$7s$
$R_{n's}(0)$	21.44	7.39	4.40
$a^{10}_{a's}$	29864.6	3548.3	1258.3

TABLE II. Values of the radial wave function at $r = 0$ in atomic units obtained by integrating numerically the Schrödinger equation, and theoretical values of a^{10}_{ns} in Mhz.

expected due to core relaxation effects on the potential. Table II shows the results.

The computer code to evaluate A and B, from the formulas described in the preceding section, has as input the quantum numbers of each LS state in the multiplet with the corresponding weight factors and the parameters a_{nl}, $a_{n',l'}$, b_{nl}, $b_{n',l'}$, theoretically calculated. The composition of the states has been taken from Reader's work [11]. The composition of the states $3/2[3/2]_1$ and $1/2[1/2]_1$ was directly calculated by using the formulas of the orthogonal transformation connecting the states $J_1 l$ and LS [9].

Table III shows the results for the values of A and B for 31 states, and some experimental results. There is no good agreement for A values in states with $n'l' = 6s$, $5d$ and $7s$. The biggest discrepancies are in the states $6s$ $3/2[3/2]_1$, $6s$ $1/2[1/2]_1$, $5d$ $^3P_1$, $5d$ $^3P_2$, $5d$ $^3D_1$, $6p$ $1/2[1/2]_1$ and $7s$ $1/2[1/2]_1$. In Reader's numerical results we can see strong configuration mixing between the states $6s$ $3/2[3/2]_1$ and $5d$ $^3P_1$, between $6s$ $1/2[1/2]_1$ and $5d$ $^3D_1$, and between $5d$ $^3P_2$, $6s$ $3/2[3/2]_2$ and $5d$ $^3D_2$; we then attribute the discrepancies to configuration mixing effects.

Sandars and Beck [4] showed that configuration superposition effects on the constants A can be taken into account by a fitting of the parameters $a_l^{k_l k_s}$ and $a_{l'}^{k_l k_s}$. In our case, each value of A depends on six such parameters when $l' \neq 0$, and on four when $l' = 0$. The number of experimental values of A is not enough to make the fit. We attempted a simpler fit, with two parameters, in the form, $A = A_l a_{nl} + A_{l'} a_{n'l'}$, that is, without calculating a_{nl} of fine structure

$5p^5n'l'$	TERM	A(Theor.)	A(Exp.)	B(Theor.)
$5p^56s$	$3/2[3/2]_2$	1524.798	1630.8709[a]	0.0780
	$3/2[3/2]_1$	1263.793	284.8028[a]	0.0389
	$1/2[1/2]_1$	3047.491	5036.5131[a]	0
$5p^55d$	$^3P_1$	−317.5979	0[a]	−0.0023
	$^3P_2$	−593.6132	147[b]	0.0084
	$^3F_4$	460.9957	376[b]	0.0735
	$^3F_3$	926.2574		0.0563
	$^3D_1$	−325.0052	350.7571[a]	−0.0291
	$^1P_1$	−1043.7520		0.0066
$5p^56p$	$3/2[1/2]_1$	891.8714	854.4084[a]	0.0029
	$3/2[5/2]_2$	1087.3760	962.3337[a]	0.0732
	$3/2[5/2]_3$	630.7050	584.59[a]; 593[b]	0.0688
	$3/2[3/2]_1$	1011.9920	794.44[a]; 793[b]	0.0084
	$3/2[3/2]_2$	699.5257		0.0073
	$1/2[3/2]_1$	3836.9340	4107.1665	0.0034
	$1/2[1/2]_1$	−997.9525	−1468.983	0.0051
	$1/2[3/2]_2$	1842.3850	1918.3850[a]	−0.0137
$5p^57s$	$3/2[3/2]_2$	1079.9070		0.0756
	$3/2[3/2]_1$	3267.360		0.0377
	$1/2[1/2]_1$	1401.921	4317.0112[a]	−0.0003
$5p^56d$	$3/2[1/2]_1$	−1087.5090		0.0074
	$3/2[7/2]_4$	432.2936		0.0770
	$3/2[3/2]_2$	175.3072		−0.0427
	$3/2[7/2]_3$	1182.3360		0.0216
	$3/2[5/2]_2$	−125.4010		−0.0636
	$3/2[5/2]_3$	370.6167		−0.0243
	$3/2[3/2]_1$	44.7940		−0.0167
	$1/2[5/2]_2$	1596.8180		0.0434
	$1/2[3/2]_2$	482.9176		−0.0529
	$1/2[5/2]_3$	610.0108		0.0662
	$1/2[3/2]_1$	−842.3018		−0.0145

TABLE III. Experimental and theoretical values of the hyperfine structure co stants A, B of Cs II in Mhz. a: from Boyd and Sawyer (1942) a Kopferman (1931), cited by Reader [11]. b: from Alvarez *et al.* (197 [8, 30, 31].

$J_1[K]_J$	A_p	A_s	a_{sp}	a_{6s}^{10}	A
$3/2[3/2]_2$	0.4218017	0.25	2685.46	2109.64	1660.14
$3/2[3/2]_1$	0.7402624	−0.0832322			1812.35
$1/2[1/2]_1$	1.739001	−0.1664640			4318.83
$^{28+1}L_J$	A_p	A_d	a_{sp}	a_{sd}	A
$^3P_2$	−0.3250626	0.7109072	2685.46	533.02	−494.01
$^3P_1$	−0.2013608	1.032186			9.42
$^3F_4$	0.2109008	0.4342301			797.81
$^3F_3$	0.4310180	0.6999884			21530.58
$^3D_1$	−0.2263469	0.1537794			211.82
$^1P_1$	−0.5834510	0.2051425			−750.01

TABLE IV. Values of a_{5p}, a_{5d}, a_{6s}^{10}, in Mhz, obtained with a two-parameter least squares fitting to seven experimental results, belonging to configurations $5p^56s$ and $5p^55d$. A_p, A_s and A_d are coefficients generated from the computer program.

intervals and a_{ns}^{10} of the wave function at the origin. Table IV shows the results obtained by using a least squares fitting [26]. There is still a difference in the states $5p^56s$ $3/2[3/2]_1$ and $5p^55d$ $^3P_2$, attributable to interaction mixing with the states $5p^56s$ $^3P_1$ and $5p^55d$ $3/2[3/2]_2$ respectively.

7. Conclusions

We obtained values of A well fitted to experiments in those states without configuration mixing, and values of B for Cs II. Unfortunately there are not experimental values for B to compare with our results. We obtained the values of radial parameters for Cs II, and of universal coefficientes coming from angular momentum considerations.

Our computer code allows the calculation of the HFS constants A, B for any atom or ion with energetic levels resulting from configurations $l^N l'$. When an atom has LS coupling, we only need the values of fine structure parameters and values of nuclear spin and dipole and quadrupole moments. If the atom has an intermediate coupling, is also required to know the composition of the states.

Our calculations show that the effective operator theory can give results well fitted to experiments in the study of HFS of Cs II. However it was not possible to test the effects of configuration mixing on the values of radial parameters because the linear equations system resulting was very unstable with the few existing experimental results, and only a two-parameter fitting was possible, but we have calculated the values neglecting configuration mixing effects.

This work shows also the lack of a theory of HFS which take into account the configuration mixing effects, as of accurate experimental determinations of factor B in Cs II.

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References

1. G. Racah, *Phys. Rev.* **61** (1942) 186; *Phys. Rev.* **62** (1942) 438; *Phys. Rev.* **62** (1942) 523; *Phys. Rev.* **76** (1949) 1352.
2. R.E. Trees,*Phys. Rev.* **92** (1953) 308.
3. C. Schwartz *Phys. Rev.* **97** (1953) 380.
4. P.G.H. Sandars and J. Beck,*Proc. Roy. Soc.* **A289** (1965) 97.
5. W.J. Childs, *Phys. Rev.* **A2** (1970) 316.
6. W.J. Childs and L.S. Goodman, *Phys. Rev.* **170** (1968) 50.

7. H. Kopferman, *Nuclear Moments in Quantum Mechanics* Ac. Press, N.Y. (1965).
8. E. Alvarez *et al.*, *Opt. Lett.* **4** (1979) 268.
9. B.G. Wybourne, *Spectroscopic Properties of Rare Earths*, Interscience, N.Y. (1965).
10. G. Racah, *Phys. Rev.* **61** (1942) 537.
11. J. Reader, *Phys. Rev.* **A13** (1976) 507.
12. H.A. Bethe and E.E. Salpeter, *Quantum Mechanics of one and two Electron Atoms*, Ac. Press, N.Y. (1957).
13. L. Armstrong, *Theory of the Hyperfine Structure of free Atoms*, Wiley, N.Y. (1971).
14. B.R. Judd, *Operator Techniques in Atomic Spectroscopy*, McGraw-Hill, N.Y. (1963).
15. B.R. Judd, *Second Quantization and Atomic Spectroscopy*, John Hopkins Press, Baltimore (1967).
16. B.R. Judd. "Group Theory in Atomic Spectroscopy". In *Group Theory and its Applications* (M. Loebl, ed.), Academic Press, New York (1968).
17. H.B.G. Casimir, *On the Interaction between Nuclei and Electrons*, Freeman, San Francisco (1963).
18. E. Fermi, in *Collected Works of Enrico Fermi*, Univ. of Chicago Press, Chicago (1965).
19. R.A. Sorensen, *Am. J. Phys.* **35** (1967) 1078.
20. J.D. Jackson, *Classical Electrodynamics*, J. Wiley, N.Y. (1969).
21. N.F. Ramsey, *Molecular Beams*, Oxford Univ. Press, Oxford (1969).
22. C. Sánchez del Río, *Introducción a la Teoría del Atomo*, Alhambra, Madrid (1977).
23. J.S. Bolemon, *Am. J. Phys.* **40** (1972) 1511.
24. V.A. Brattsev, *Tables of Atomic Wave Functions*, Science Publishing House, Moscow (1966).
25. D. Hartree, *Calculation of Atomic Structures*, J. Wiley, N.Y. (1957).
26. F. Scheid, *Análisis Numérico*, McGraw-Hill, México (1972).
27. A.R. Edmonds, *Angular Momentum in Quantum Mechanics*, Princeton Univ. Press, Princeton (1957).
28. C.W. Nielson and G.F. Koster, *Spectroscopic Coefficients for the p^n, d^n and f^n configurations*, MIT Press, Cambridge (1963).
29. C.E. Moore, *Atomic Energy Levels*, Nat. B of St. Circ. 467, vol. III, Washington D.C. (1958).

30. A. Bengtson *et al.*, *Phys. Lett.* **76A** (1980) 45.
31. E. Alvarez *et al.*, *Phys. Rev.* **A 21** (1980) 710.
32. W.J. Childs, *Phys. Rev.* **156** (1967) 71.
33. A. Kastler, *J. Phys.* **11** (1950) 255.