

## Off-diagonal hyperfine interaction and parity nonconservation in cesium

V. A. Dzuba and V. V. Flambaum

*School of Physics, University of New South Wales, Sydney 2052, Australia*

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We have performed relativistic many-body calculations of the hyperfine interaction in the  $6s$  and  $7s$  states of Cs, including the off-diagonal matrix element. The calculations were used to determine the accuracy of the semiempirical formula for the electromagnetic transition amplitude  $\langle 6s|M1|7s\rangle$  induced by the hyperfine interaction. We have found that even though the contribution of the many-body effects into the matrix elements is very large, the square-root formula  $\langle 6s|H_{hfs}|7s\rangle = \sqrt{\langle 6s|H_{hfs}|6s\rangle\langle 7s|H_{hfs}|7s\rangle}$  remains valid to the accuracy of a fraction of  $10^{-3}$ . The result for the  $M1$ -amplitude is used in the interpretation of the parity-violation measurement in the  $6s-7s$  transition in Cs, which claims a possible deviation from the standard model.

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### I. INTRODUCTION

Recent progress in highly accurate measurements of parity nonconservation (PNC) in atoms has got to the point where new physics beyond the standard model of elementary particles can be studied. The latest analysis [1] of the most precise measurements of the PNC in cesium [2] suggests that the value of the weak charge of the  $^{133}\text{Cs}$  nucleus may differ from the prediction of the standard model. In that experiment [2], the ratio of the PNC  $E1$  amplitude to the tensor polarizability  $\beta$  for the  $7S_{1/2}-6S_{1/2}$  transition was measured with 0.35% accuracy. The measured value can be written in the form

$$\frac{k_{PNC}}{\beta} \frac{Q_W}{N}, \quad (1)$$

where  $k_{PNC}$  is the electron matrix element of the electric dipole transition induced by the weak interaction between  $7S_{1/2}$  and  $6S_{1/2}$  states of  $^{133}\text{Cs}$ ,  $Q_W$  is the weak nuclear charge and  $N$  is the number of neutrons. To interpret the measurements in terms of the weak nuclear charge one needs to know  $k_{PNC}$  and  $\beta$ . The value of  $k_{PNC}$  can be obtained from atomic calculations only. Bennett and Wieman [1] used the value  $k_{PNC}=0.9065(36)iea_0$ , which is the average of our result  $k_{PNC}=0.908(9)iea_0$  [3] obtained in 1989 and the result of the Notre Dame group  $k_{PNC}=0.905(9)iea_0$  [4] obtained in 1990. Note that Bennett and Wieman assumed 0.4% accuracy of the calculations contrary to the 1% accuracy claimed in both calculations. This assumption was based on the comparison of the calculated atomic quantities relevant to the PNC amplitude (electromagnetic transition amplitudes between lower  $s$  and  $p$  states and hyperfine structure intervals of these states) with the latest very accurate measurements, which resolved major discrepancies between theory and experiment in favor of theory.

The most precise value of  $\beta$ ,  $\beta=27.024(43)(67)a_0^3$ , was obtained in Ref. [1] from the measurements of the ratio  $M1_{hfs}/\beta$  where  $M1_{hfs}$  is the  $M1$  transition amplitude between the states  $6S$  and  $7S$  induced by the hyperfine structure (hfs) interaction. The semiempirical formula for the  $M1_{hfs}$  amplitude derived in Refs. [5–7] was used in the analysis:

$$M1_{hfs} = - \left| \frac{\mu_B}{c} \right| \frac{\sqrt{A_{6s}A_{7s}}}{|E_{7s}-E_{6s}|} \frac{1}{2} (g_s - g_I) 1.0024. \quad (2)$$

Here  $A_{6s}$  and  $A_{7s}$  are the hfs constants of the  $6s$  and  $7s$  states of Cs,  $g_s=2.0025$ ,  $g_I=-0.0004$ , the coefficient 1.0024 was introduced to account for the many-body effects. This gives  $M1_{hfs} = |\mu_B/c| 0.8094(20) \times 10^{-5}$  [6,7].

Values  $\beta=27.024(43)(67)a_0^3$  and  $k_{PNC}=0.9065(36)iea_0$  and measurements of Eq. (1) [2] lead to the value of the weak charge of  $^{133}\text{Cs}$   $Q_W = -72.06(28)(34)$  which differs from the prediction of the standard model  $Q_W = -73.20(13)$  [8] by  $2.5\sigma$ .

From the point of view of accurate atomic calculations, there are two major questions in the analysis above that should be considered. The first is whether the actual accuracy of the PNC calculations is really 0.4%. The second is whether the semiempirical formula (2) is accurate. In the present paper we address the second question, leaving the first one for later work.

### II. PRELIMINARY ANALYSIS

$M1_{hfs}$  amplitude appears due to mixing of the  $6s$  and  $7s$  states by the hfs interaction,

$$M1_{hfs} = \frac{\langle 6s, F | H_{hfs} | 7s, F \rangle}{E_{6s} - E_{7s}} \langle 7s, F | M1 | 7s, F' \rangle + \langle 6s, F | M1 | 6s, F' \rangle \frac{\langle 6s, F' | H_{hfs} | 7s, F' \rangle}{E_{6s} - E_{7s}}. \quad (3)$$

Two major assumptions have been made to arrive at Eq. (2) from Eq. (3). First, the nonrelativistic expression for the operator of the  $M1$  transition was used:

$$M1 = -|\mu_B|g(\mathbf{L} + 2\mathbf{S}). \quad (4)$$

Second, the square-root formula is assumed to be valid

$$\langle 6s | H_{hfs} | 7s \rangle = \sqrt{\langle 6s | H_{hfs} | 6s \rangle \langle 7s | H_{hfs} | 7s \rangle}. \quad (5)$$

The accuracy of both of these assumptions needs to be examined. The situation is clear with the relativistic corrections to the  $M1$  operator (4). According to the estimations of Bou-

chiat and Piketty [6] the relativistic effects modify the amplitudes  $\langle 6s|M1|6s\rangle$  and  $\langle 7s|M1|7s\rangle$  at only the  $10^{-4}$  level. This is in line with the many-body calculations of the relativistic effects in  $g$  factors and  $M1$ -transition amplitudes for C's and other alkali atoms in our early works [9,10].

The situation with the square-root formula (5) is less clear. In their pioneering work Bouchiat and Piketty [6] estimated the first-order core polarization corrections to it and introduced the correction factor 1.0017. In a later paper by Bouchiat and Guéna [7] this factor was assumed to be 1.0024 [see also formula (2)]. The accuracy of the estimation of the many-body correction was assumed to be approximately equal to the correction itself ( $\sim 0.002$ ) [6,7]. In these works there were no accurate calculations of other many-body contributions to the hfs beyond the first-order core polarization corrections. However, it is known that these contributions can be up to 20% of the hyperfine structure (see below). The applicability of Eq. (2) in this situation is not obvious.

The accurate relativistic many-body calculations of the off-diagonal hfs matrix element (5) were recently performed by the Notre Dame group [11]. The accuracy of the calculations was about 1% and agreement with formula (5) within this accuracy was achieved. Note that the theoretical accuracy for the diagonal hfs matrix elements is also about 1% (see Refs. [12] and [13] and this paper). This accuracy is not sufficient to find an accurate value of  $\beta$  to add anything new to the result of the cesium PNC experiment published in Ref. [2].

However, we believe that the validity of the square-root formula (5) can be demonstrated to much higher accuracy than the absolute theoretical accuracy of the hfs calculations (here we agree with Refs. [5–7]). We suggest that the following combination of matrix elements be calculated

$$R = \frac{\langle 6s|H_{hfs}|7s\rangle}{\sqrt{\langle 6s|H_{hfs}|6s\rangle\langle 7s|H_{hfs}|7s\rangle}} - 1, \quad (6)$$

where all hfs matrix elements are calculated in the same approximation. The value of  $R$  can be calculated with very high accuracy because uncertainties in different matrix elements cancel each other almost exactly. We will demonstrate that inclusion of different many-body and relativistic effects leave the formula

$$\langle 6s|H_{hfs}|7s\rangle = \sqrt{\langle 6s|H_{hfs}|6s\rangle\langle 7s|H_{hfs}|7s\rangle} \quad (7)$$

valid to very high accuracy, so that the value of  $R$  (6) remains very small.

Let us start from the analytical estimates of different contributions to  $R$  in Eq. (6). First note that in the single-electron approximation, formula (7) is exact if the wave functions of the  $6s$  and  $7s$  states are proportional:

$$\psi_{6s} = B\psi_{7s} \quad (8)$$

( $a_0$  is Bohr radius) at short distances from the nucleus,  $r \leq a_0/Z$ . Dirac equations for the states  $6s$  and  $7s$  differ by the energy only. Therefore, their solutions at short distances,

where the difference in energies is small compared to the potential, differ by normalization only. One can say that Eq. (8) is valid if

$$\Delta E/|V| \ll 1, \quad (9)$$

where  $\Delta E = 0.08445$  a.u. is the energy difference between the  $6s$  and  $7s$  states of Cs and  $V$  is the atomic potential. The Hamiltonian of the hfs interaction  $H_{hfs}$  is proportional to  $1/r^3$  and the main contribution to its matrix elements comes from the distances  $r \leq a_0/Z$ . Substitution of  $V = Ze^2/r$ ,  $r = a_0/Z$ , and  $Z = 55$  into Eq. (9) gives

$$\frac{\Delta E}{V} \approx 3 \times 10^{-5}. \quad (10)$$

Note that for  $s$  waves the correction can be even smaller. Indeed, in the nonrelativistic approximation,  $s$ -wave hfs is proportional to  $\delta(r)$ . Thus, the typical distances  $r \sim \hbar/(m_e c) = \alpha a_0$ , where  $\alpha = 1/137$ .

Let us now consider the many-body effects. It is convenient to do this using the many-body perturbation theory in the residual Coulomb interaction  $U$ ,  $U = H - H_{HF}$ . Here  $H$  is the exact Hamiltonian of the atom and  $H_{HF}$  is the Hartree-Fock Hamiltonian. We generate the complete zero-approximation set of the eigenvalues, wave functions, and Green's functions using the Hartree-Fock Hamiltonian. The small parameter of this many-body perturbation theory is the ratio of the nondiagonal matrix element of the residual interaction  $U$  to the large energy denominator for excitation of the electron from the closed electron shell (electron core), e.g.,  $5p$  electron:  $U/E_{5p} \sim 10^{-2}$ .

The perturbative (correlation) corrections to the hfs matrix element can be divided into two classes: the self-energy corrections and the vertex corrections. The former can be included into Eq. (6) through the redefinition of the single electron wave functions while the latter are included through the redefinition of the  $H_{hfs}$  operator.

Self-energy corrections dominate in the hfs of alkali atoms (see, e.g., Ref. [14]). The major contribution is due to the correlations between an external electron and core electrons. We include them by using so-called Brueckner orbitals instead of the Hartree-Fock orbitals as the single-electron wave functions in Eq. (6). The Brueckner orbitals are obtained by introducing an additional operator  $\hat{\Sigma}$  into the Hartree-Fock equations for the external electron and solving the Dyson-type equation  $[H_{HF} + \hat{\Sigma}(E) - E]\psi = 0$ . The  $\hat{\Sigma}$  is an energy-dependent nonlocal operator, which is also called the ‘‘correlation potential’’ [12,15]. For the calculation of  $\hat{\Sigma}$ , see the next section. The Brueckner type correlation correction constitutes 20% of the hfs of  $6s$  and  $7s$  states of Cs. However, if we neglect the dependence of  $\hat{\Sigma}$  on energy, the estimation (10) is still valid. It follows from the calculations that  $\partial\hat{\Sigma}/\partial E \sim 1\%$  for  $E \sim E_{6s}, E_{7s}$  (it is suppressed by the parameter  $\Delta E/E_{5p}$ ). This leaves condition (10) practically unchanged.

Dominating vertex corrections to the hfs matrix element are due to the effect of core polarization by the nuclear di-

pole magnetic field. Since the core states change in the magnetic field, the Hartree-Fock potential  $V$  created by the core electrons, as well as the correlation potential  $\Sigma$ , also change. The effect of this change on the hfs can be accounted for by redefining the operator of the hfs interaction [12]:

$$H'_{hfs} = H_{hfs} + \delta V + \delta \Sigma. \quad (11)$$

The correction to the hfs caused by  $\delta V$  is often called the random-phase approximation (RPA)-type [16] correction, while another correction associated with  $\delta \Sigma$  is the non-Brueckner correlation correction or structural radiation [15]. These corrections are more likely to cause deviation from the square-root formula since they are localized on larger distances up to the core radius. Note, however, that in the case of the hfs interaction  $\delta V$  is completely due to the Hartree-Fock exchange potential. There is no change to the Hartree-Fock direct potential since the magnetic field does not change electron density in the first order of perturbation theory. This means that  $\delta V$  vanishes exponentially outside the core. Inside the core, at  $r \sim a_0$ ,  $\Delta E/V \sim 0.01$  and the  $6s$  and  $7s$  orbitals are still proportional. Note that the potential  $V$  at these distances may be estimated as  $V \sim -Z_{eff}e^2/r$ , where  $Z_{eff} \sim 5$ . Since the contribution of  $\delta V$  is about 10%, we come to the estimate  $10^{-3}$  for the error of the square-root formula.

There is one more reason why the square-root formula is accurate. The expression for  $R$  [Eq. (6)] is symmetric with respect to the energies  $E_{6s}$  and  $E_{7s}$ . Therefore, its expansion in  $\Delta E$  ( $\Delta E = E_{6s} - E_{7s}$ ) starts from  $\Delta E^2$ :

$$R = a(\Delta E)^2 + b(\Delta E)^4 + \dots \quad (12)$$

Since all linear in  $\Delta E$  terms are canceled out, one can say that the error should be smaller than in the estimates above. The dimensionless parameter for Eq. (12) is

$$(\Delta E/E_{5p})^2 \sim 10^{-2},$$

where  $E_{5p} \approx 0.84$  a.u. is the core excitation energy. Since the term  $a(\Delta E)^2$  arises due to  $\delta V$  and  $\delta \Sigma$ , which contribute about 10% and 1%, respectively, into the hfs, the total deviation from the square-root formula caused by the RPA and non-Brueckner corrections should be smaller than  $10^{-1} \times 10^{-2} = 10^{-3}$ . We may add that the contribution of  $\delta \Sigma$  to the hfs is much smaller than the contribution of  $\Sigma$  since  $\delta \Sigma$  has an additional suppression by the parameter  $(\Delta E/E_{5p})$  [15].

There are also contributions to the self-energy and vertex due to the radiative corrections. We have not considered these contributions in our calculations. However, they come from the very short distances  $r \leq \hbar/m_e c = \alpha a_0$  and should not cause any significant deviation from the square-root formula.

Finally, let us estimate contributions to  $M1_{hfs}$ , which cannot be presented in the form of Eq. (3). Let us use the basis of the exact atomic eigenstates and treat  $H_{hfs}$  as a perturbation in this basis. The result can be presented in the form

$$M1_{hfs} = \sum_{\alpha} \frac{\langle \widetilde{6s}, F | H_{hfs} | \alpha, F \rangle}{E_{6s} - E_{\alpha}} \langle \alpha, F | M1 | \widetilde{7s}, F' \rangle + \sum_{\beta} \frac{\langle \widetilde{6s}, F | M1 | \beta, F' \rangle \langle \beta, F' | H_{hfs} | \widetilde{7s}, F' \rangle}{E_{\beta} - E_{7s}}. \quad (13)$$

Here  $|\widetilde{6s}\rangle, |\widetilde{7s}\rangle, |\alpha\rangle, |\beta\rangle$  are the eigenstates that include all possible configuration mixing,  $|\alpha\rangle$  and  $|\beta\rangle$  may contain an arbitrary number of pairs of excited electrons and holes in the electron core. All nondiagonal matrix elements of the  $M1$  operator vanish in the nonrelativistic limit. Moreover, it was demonstrated in our paper [9] that the dominant contribution appears only in the second order in the spin-orbit interaction and in the first order in configuration mixing, i.e., nondiagonal  $M1$  matrix elements are of the order  $M1 \sim (Z\alpha)^4 Q_{in}/E \sim 10^{-4} - 10^{-5} |\mu_B|$ , where  $Q_{in}$  is the nondiagonal matrix element of the Coulomb interaction corresponding to an excitation of a core electron and  $E$  is the energy of this excitation. Indeed, the operator of the magnetic moment is  $M1 = \mu_B(\mathbf{L} + 2\mathbf{S}) = \mu_B(2\mathbf{J} - \mathbf{L})$  (relativistic correction to this expression  $\sim 10^{-5}$ ). Electron wave functions are the eigenfunctions of the total electron angular momentum  $\mathbf{J}$ . Therefore,  $\mathbf{J}$  does not give any nondiagonal matrix elements. On the other hand, the matrix element  $\langle \alpha, J = 1/2 | \mathbf{L} | \beta, J = 1/2 \rangle$  requires spin-orbit interaction both in the bra  $\langle \alpha, J = 1/2 |$  and ket  $|\beta, J = 1/2 \rangle$  vectors, since in the nonrelativistic limit they correspond to the total orbital angular momentum  $L = 0$ , i.e.,  $\mathbf{L}|\alpha\rangle = \mathbf{L}|\beta\rangle = 0$ . Thus, we need the second order in spin-orbit interaction. Note that the nondiagonal in angular momentum  $L$  matrix elements of the hyperfine interaction like  $\langle \widetilde{s}_{1/2} | H_{hfs} | \widetilde{d}_{3/2} \rangle$  do not help since in this case both the hfs matrix element and  $M1$  matrix element  $\langle \widetilde{s}_{1/2} | M1 | \widetilde{d}_{3/2} \rangle$  are very small.

Nondiagonal matrix elements of  $M1$  were calculated in Refs. [9] and [10]; the value  $\langle 6s | M1 | 7s \rangle \approx 0.4 \times 10^{-4} |\mu_B|$  was measured in Refs. [17], [5] and [18]. Thus, each term with the nondiagonal  $M1$  matrix element in Eq. (13) is suppressed by a factor of  $10^{-4} - 10^{-5}$ . Therefore, we may safely assume that the correction to the diagonal  $M1$  contribution (3) does not exceed  $10^{-3}$ .

We should note that it may not be easy to come to this conclusion using perturbation theory in the Dirac basis of electron orbitals ( $jj$  scheme) (Dirac basis was used in Ref. [6]). In this basis the small result must appear due to strong cancellations between different terms in the sum over intermediate states.

### III. MANY-BODY CALCULATIONS

To test the validity of the square-root formula (7) we performed accurate many-body relativistic calculations of the off-diagonal and diagonal hfs matrix elements. Detailed discussion of the accurate hfs calculations can be found elsewhere [12]. Here we repeat the main points emphasizing the role of different many-body effects.

We start calculations from the relativistic Hartree-Fock

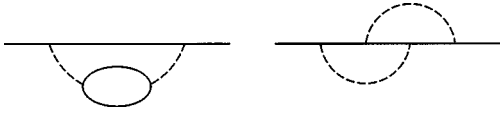


FIG. 1. Second-order diagrams for the self-energy of the valence electron ( $\hat{\Sigma}$  operator). Dashed line is the Coulomb interaction between core and valence electrons. Loop is the polarization of the atomic core, which corresponds to the virtual creation of the excited electron and a hole in the core shells.

method in the  $V^{N-1}$  approximation (calculations for the external electron are carried out in the frozen self-consistent field of the core). The core polarization is calculated using the Hartree-Fock equations in an external field [14]. It is equivalent to the well-known random-phase approximation with exchange method (see, e.g., Ref. [16]). The many-body effects such as the Brueckner-type correlations, and the structural radiation are included by means of the correlation potential method [15]. As it was pointed out in the previous section, the Brueckner-type correlation corrections are included by solving the Dyson-type equation for the states of the external electron

$$(H_{HF} + \hat{\Sigma} - E)\psi = 0. \quad (14)$$

Correlation potential  $\hat{\Sigma}$  accounts for the correlation between an external electron and core electrons. We use many-body perturbation theory and the Feynman diagram technique to calculate  $\hat{\Sigma}$  [12,19]. The perturbation expansion of  $\hat{\Sigma}$  in the residual Coulomb interaction starts from the second order. The corresponding diagrams are presented in Fig. 1. We include both the second-order diagrams and three dominating classes of higher-order correlations:

(1) Screening of the Coulomb interaction between an external electron and core electrons by other core electrons—This is a collective phenomenon and the corresponding chain of diagrams is enhanced by a factor approximately equal to the number of electrons in the external closed subshell (the  $5p$  electrons on Cs). We stress that our approach takes into account screening diagrams with double, triple, and higher core electron excitations in contrast to the popular coupled cluster method where only double and selected triple excitations are considered (see, e.g., Ref. [13]). The effect of screening is taken into account in all orders by summation of the corresponding chain of diagrams, which in the Feynman diagram technique form a matrix geometrical progression.

(2) Hole-particle interaction in the core polarization operator—This effect is enhanced by the large zero-multipolarity diagonal matrix elements of the Coulomb inter-

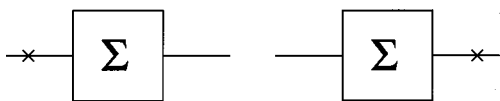


FIG. 2. Brueckner-type correlation diagrams for the hfs. Cross denotes the hfs interaction. The  $\Sigma$  operator includes second-order diagrams (Fig. 1) and higher-order diagrams as described in the text.

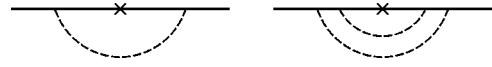


FIG. 3. Core polarization (RPA) diagrams for the hfs in the first and second order in Coulomb interaction.

action. We take it into account by amending the direct Hartree-Fock potential in which the polarization operator is calculated.

(3) Iterations of the self-energy operator ( $\hat{\Sigma}$ )—This chain of diagrams describes the nonlinear effects of the correlation potential and is enhanced by the small denominator, which is the excitation energy of an external electron (in comparison with the excitation energy of a core electron). The iterations of  $\hat{\Sigma}$  are included by solving Eq. (14).

Substituting the Brueckner orbitals into Eq. (6) accounts for the dominating correlation corrections to the hfs. Corresponding diagrams are presented in Fig. 2. These corrections constitute 23% of the hfs of the  $6s$  state of Cs and 12% of the hfs of the  $7s$  state of Cs.

To take into account the core polarization effect we self-consistently solve the Hartree-Fock equation for the core states in the nuclear magnetic field. The details are presented in Ref. [14]. When all corrections  $\delta\psi_n$  to core states caused by the magnetic field are found, they are used to calculate the correction  $\delta V$  to the Hartree-Fock potential. Then core polarization is included into the single-electron matrix element  $\langle a | H_{hfs} | b \rangle$  between valence states  $|a\rangle$  and  $|b\rangle$  by redefining the operator of the hfs interaction  $H'_{hfs} = H_{hfs} + \delta V$ . This corresponds to the summation of the infinite series of the RPA-type of diagrams presented in Fig. 3. The RPA-type core polarization contribution to the hfs of the  $6s$  and  $7s$  states of Cs is about 15%.

Core polarization also leads to the change of  $\hat{\Sigma}$ . Corresponding contributions to the hfs matrix element  $\langle a | \delta\hat{\Sigma} | b \rangle$  are often called structural radiation. Second-order diagrams for structure radiation are presented in Fig. 4. We use direct summation over the complete set of single-electron states to calculate these diagrams.

There is also a contribution to the hfs due to the change of normalization of the wave function caused by  $\hat{\Sigma}$ . This contribution can be written in a form

$$A_{norm} = \frac{1}{2} \langle a | H_{hfs} | b \rangle (\langle a | \partial\hat{\Sigma} / \partial E | a \rangle + \langle b | \partial\hat{\Sigma} / \partial E | b \rangle). \quad (15)$$

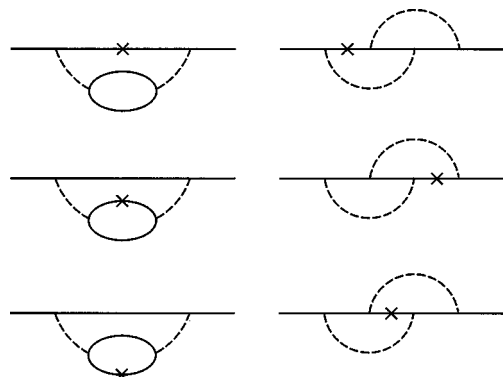


FIG. 4. Structural radiation.

TABLE I. Hyperfine structure matrix elements for the  $6S$  and  $7S$  states of  $^{133}\text{Cs}$  (MHz).

Approximation		$A_{6S}$	$A_{7S}$	$\sqrt{A_{6S}A_{7S}}$	$\langle 6S h 7S \rangle$	$\frac{\langle 6S h 7S \rangle}{\sqrt{A_{6S}A_{7S}}} - 1$
$\psi = \psi_{HF}$	$\langle \psi h \psi \rangle$	1424.8	391.5	746.9	746.9	0
	$\langle \psi h + \delta V \psi \rangle$	1712.5	469.7	896.9	897.1	$2.2 \times 10^{-4}$
	$\langle \psi h + \delta V + \delta \Sigma \psi \rangle$	1687.8	466.9	887.7	887.6	$1.1 \times 10^{-4}$
$\psi = \psi_{Br}$	$\langle \psi h \psi \rangle$	1952.4	459.5	947.2	947.2	0
	$\langle \psi h + \delta V \psi \rangle$	2302.0	541.4	1116.3	1116.7	$3.5 \times 10^{-4}$
	$\langle \psi h + \delta V + \delta \Sigma \psi \rangle$	2267.6	537.7	1104.3	1104.5	$1.8 \times 10^{-4}$
$\psi = \psi_{jit}$ <sup>a</sup>	$\langle \psi h + \delta V \psi \rangle$	2308.3	542.5	1119.0	1119.5	$4.4 \times 10^{-4}$
	$\langle \psi h + \delta V + \delta \Sigma \psi \rangle$	2273.8	538.8	1106.9	1107.3	$3.6 \times 10^{-4}$
	SDpT <sup>b</sup>	2278.5	540.6	1109.8		
Experiment <sup>c</sup>		2298.2	545.9	1120.1		

<sup>a</sup>Brueckner orbitals with  $\Sigma$  operator rescaled to fit the energy.

<sup>b</sup>Single, double, and partly triple excitation approximation; calculations by the Notre Dame group, Ref. [13].

<sup>c</sup>Reference [20].

The combined contribution of the structural radiation and renormalization into the hfs of the  $6s$  and  $7s$  states of Cs are 1.5% and 0.6%, respectively.

When all dominating higher-order correlations are included into the calculation of the Brueckner orbitals for the  $6s$  and  $7s$  states of cesium, the accuracy for the calculated energies of these states is very high and constitutes about 0.1%. However, we introduced fitting parameters to rescale  $\Sigma$  to fit the energies exactly. This procedure allows us to effectively include some omitted higher-order correlations and to test the sensitivity of the hfs matrix elements to the value of  $\Sigma$ .

The results for the hfs are presented in Table I. In this table  $h \equiv H_{hfs}$ , the matrix elements of  $\delta V$  are RPA-type corrections, the matrix elements of  $\delta \Sigma$  are structural radiation [including renormalization (15)] matrix elements with  $\psi_{Br}$  and include Brueckner-type correlation corrections. One can see that the correction to the square-root formula due to the considered many-body effects does not exceed  $4.4 \times 10^{-4}$ . When all dominating many-body effects are taken into account, the accuracy of the calculated hfs constants compared to experiment is about 1%. However the square-root formula is still valid to the accuracy of about  $10^{-4}$ . The most likely cause of the remaining discrepancy with experiment is higher-order correlation corrections not included in our calculations. These corrections are localized on the radius of the core and due to the fact that these corrections are very small ( $\sim 1\%$  of the experimental hfs) it is extremely unlikely that they can break the square-root formula. The same may be said about the very small radiative and Breit corrections. Note that our final results for the diagonal hfs matrix elements for the  $6s$  and  $7s$  states are in very good agreement with the calculations of the Notre Dame group [13].

It follows from the above, that the correction to the square-root formula is about an order of magnitude smaller than the estimations of Bouchiat and Guéna [7]. However,

there is no formal disagreement between the results, since Bouchiat and Guéna estimated the uncertainty of their result to be equal to the correction itself. We believe that for the analysis of the PNC experiment it is safer to assume no correction to the square-root formula. This slightly changes the numbers. The  $M1_{hfs}$  amplitude, tensor polarizability  $\beta$ , and weak charge of the  $^{133}\text{Cs}$  nucleus become

$$M1_{hfs} = \left| \frac{\mu_B}{c} \right| 0.8074(8) \times 10^{-5},$$

$$\beta = 26.957(43)(27)a_0^3, \quad (16)$$

$$Q_W = -71.88(28)(29).$$

To stress the importance of the result here we used an estimate of the theoretical accuracy 0.4% [1] in the value of  $k_{PNC}$ . Our result for  $M1_{hfs}$  is in very good agreement with the result of Derevianko *et al.* [11]

$$M1_{hfs} = \left| \frac{\mu_B}{c} \right| 0.8070(73) \times 10^{-5}, \quad (17)$$

but has better accuracy. The weak nuclear charge  $Q_W$  in Eq. (16) represents even larger deviation from the standard model value  $Q_W = -73.20(13)$  [8] than the result presented by Bennett and Wieman [1]. The deviation is  $2.9\sigma$  if 0.4% accuracy of calculations of the  $k_{PNC}$  is assumed. Note that even if 1% accuracy is assumed for the calculated value of  $k_{PNC}$ , as it was claimed in both theoretical works [3,4], then there is still  $1.5\sigma$  deviation from the standard model. However, we would like to stress once more that before making any conclusions about agreement or disagreement with the standard model the question about the accuracy of the atomic calculations of the PNC electronic matrix element  $k_{PNC}$  [see Eq. (1)] should be carefully reanalyzed.

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