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Multiconfiguration Dirac-Hartree-Fock calculations for the hyperfine-structure parameters and the scalar-pseudoscalar interaction constant of ^{133}Cs

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Abstract. In this work we investigate the applicability of the multiconfiguration Dirac-Hartree-Fock (MCDHF) method for calculating parity and time reversal symmetry violations in many-electron atoms. As an example we show results from calculations of the scalar-pseudoscalar interaction constant for ^{133}Cs. Calculated limits of this interaction constant are in a good agreement with other theories.

1. Introduction

The observation of a static electric dipole moment (EDM) of a many-electron atom which violates parity, P, and time reversal, T, symmetry, may be a very important step in searching for a new physics beyond the Standard model of elementary particles [1, 2]. One of the main possible sources of EDM in the paramagnetic atoms is the scalar - pseudoscalar ($S-PS$) interaction between the electrons and the nucleus:

$$\hat{H}_{S-PS} \;=\; i\frac{G_F}{\sqrt{2}}\, C_{S-PS}\, A \sum_{j=1}^{N} \beta_j\, \gamma_j^5\, \rho\,(r_j)\,. \tag{1}$$

Here G_F is the Fermi constant, C_{S-PS} is the $S-PS$ interaction constant, A is the mass number, β and γ^5 are the Dirac matrices and $\rho(r)$ is the nuclear density function. The interaction mixes parity of atomic states and also induces a static electric dipole moment of the atom. A number of calculations have previously been done using various types of perturbation theories and coupled cluster methods [1]. The aim of this work was to investigate the applicability of the multi-configuration Dirac-Hartree-Fock (MCDHF) method for calculating parity and time reversal symmetry violations in many-electron atoms, and as a test case we consider the mixture of $\left|6s\ ^2S_{1/2}\right\rangle$ and $\left|6p\ ^2P_{1/2}\right\rangle$ atomic states in ^{133}Cs.

2. MCDHF method for parity and time reversal symmetry violations

In the MCDHF method an atomic state function (ASF) is obtained as the linear combination of configuration state functions (CSFs) with same parity, P, total angular momentum of electrons, J, and one of its projections, M_J [3]:

$$\Psi\left(\gamma PJM_J\right) \;=\; \sum_{r=1}^{n} c_r \Phi\left(\gamma_r PJM_J\right). \tag{2}$$

The P and T symmetry violations induced by $S-PS$ interaction include small admixtures of the opposite parity at the same angular momentum and one of its projections to the main ASF [4]:

$$\widetilde{\Psi}\left(\gamma JM_J\right) \;=\; a\Psi\;\left(\gamma PJM_J\right) \;+\; \sum_{i=1}^{m} b_i\;\Psi\left(\alpha_i(-P)JM_J\right). \tag{3}$$

The scalar-pseudoscalar interaction is very weak and the coefficient a of the dominant component can, to a good approximation, be set to unity. The mixing coefficients (a, b_i) are obtained after the diagonalization of the full atomic Hamiltonian ($\hat{H}_A \;=\; \hat{H}_{DC} \;+\; \hat{H}_{S-PS}$) matrix. Atomic state functions $\widetilde{\Psi}\left(\gamma JM_J\right)$ with mixed parity can be used for calculating the static electric dipole moment, D_A,

$$D_A \;=\left\langle \widetilde{\Psi}\left(\gamma JM_J\right)|\hat{D}_Z|\widetilde{\Psi}\left(\gamma JM_J\right)\right\rangle = \;2a\;\sum_{i=1}^{m} b_i \left\langle \Psi\;\left(\gamma PJM_J\right)|\hat{D}_Z|\Psi\left(\alpha_i(-P)JM_J\right)\right\rangle, \tag{4}$$

where $\hat{D}_Z$ is the z-projection of the electric dipole moment operator. In accordance with the experiments for the spin-polarized atoms it is assumed that $M_J \;=\; J$. By combining experimentally obtained limits of D_A with calculated matrix elements, the limit of the constant C_{S-PS} can be found.

3. Evaluation of matrix elements

According to the Wigner-Eckart theorem a matrix element of general tensor operator $\hat{T}^k_q$ can be expressed as:

$$\begin{aligned}&\left\langle \Psi\;\left(\gamma PJM_J\right)|\hat{T}^k_q|\Psi\left(\alpha(-P)JM_J\right)\right\rangle \\ &\qquad = (-1)^{J-M_J}\begin{pmatrix} J & k & J \\ -M_J & q & M_J\end{pmatrix}\sqrt{2J+1}\;\left[\Psi\;\left(\gamma PJ\right)\|\hat{T}^k\|\Psi\left(\alpha(-P)J\right)\right].\end{aligned} \tag{5}$$

Using multiconfiguration expansions (2) the reduced matrix elements between the ASFs can be written:

$$\left[\Psi\;\left(\gamma PJ\right)\|\hat{T}^k\|\Psi\left(\alpha(-P)J\right)\right] \;=\; \sum_{r,s} c_r c_s\left[\Phi\;\left(\gamma_r PJ\right)\|\hat{T}^k\|\Phi\left(\gamma_s(-P)J\right)\right], \tag{6}$$

where reduced matrix elements of the one-electron operator between CSFs can be expressed as sums over elements involving single-particle orbitals [5]:

$$\left[\Phi\;\left(\gamma_r PJ\right)\|\hat{T}^k\|\Phi\left(\gamma_s(-P)J\right)\right] = \;\sum_{a,b} d_{ab}(rs)\left[n_a\kappa_a\|\hat{t}^k\|n_b\kappa_b\right]. \tag{7}$$

The single-particle reduced matrix elements $\left[n_a\kappa_a\|\hat{t}^k\|n_b\kappa_b\right]$, in turn, can be factorized into reduced angular matrix elements and radial integrals. Here we give the factorization of the

single-particle matrix elements corresponding to the $\hat{H}_{S-PS}$ interaction operator ($k = 0$, $q = 0$) and the $\hat{D}_Z$ electric dipole moment operator ($k = 1$, $q = 0$):

$$\left[n_a\kappa_a\|\hat{h}_{S-PS}\|n_b\kappa_b\right] = \delta\left(-\kappa_a,\kappa_b\right)\frac{G_F}{\sqrt{2}}C_{S-PS}\;A\int_0^\infty \rho\left(r\right)\left(P_aQ_b\;-\;P_bQ_a\right)\;dr. \quad (8)$$

$$\left[n_a\kappa_a\|\hat{d}^1\|n_b\kappa_b\right] = -\left[\kappa_a\|C^1\|\kappa_b\right]\int_0^\infty \left(P_aP_b\;+\;Q_aQ_b\right)\;r\;dr. \quad (9)$$

For the calculations of the matrix elements we extended the GRASP relativistic atomic structure package [6]. The extension, presented in this work, includes programs for both $S-PS$ and electric dipole matrix elements. The nuclear density function, $\rho(r)$, was modeled as a Fermi distribution.

4. MCDHF calculations

For the MCDHF expansions of the even and odd ASFs we used several models. In the first model the CSFs are obtained from single substitutions from all orbitals of the main configuration to an increasing active set (AS) of orbitals. The energy functional on which the orbitals are optimized is defined according to an extended optimal level (EOL) scheme, where a linear combination of two atomic states (even and odd) is used. CSFs of the second model additionally include double core-core and core-valence substitutions from the $4s$, $4p$, $4d$, $5s$, $5p$, $6s$, $6p$ orbitals without relaxation (using one-electron radial functions obtained in the first model without re-optimization) in relativistic configuration interaction calculations. The AS is labeled by an integer n and includes s, p, d orbitals with principal quantum numbers up to n and f orbitals up to $n-1$. For example, the active set $AS_{n=8}$ contains s, p, d orbitals with principal quantum numbers up to $n = 8$ and f orbitals up to $n = 7$. The active sets were successively extended to $n = 13$. At all steps in the first model only new orbitals are optimized.

The calculated energy differences (in cm^{-1}) between the two atomic states $\left|6s\ ^2S_{1/2}\right\rangle$ and $\left|6p\ ^2P_{1/2}\right\rangle$ of ^{133}Cs are displayed in Table 1. The included core-valence and core-core effects of the second model improve the energy difference substantially compared to the simple single-excitation model.

Table 1 Calculated energy differences (in cm^{-1}) between $\left|6s\ ^2S_{1/2}\right\rangle$ and $\left|6p\ ^2P_{1/2}\right\rangle$ in the two models as functions of the active set.

AS	$E_{6p}\ -\ E_{6s}$ (1)	$E_{6p}\ -\ E_{6s}$ (2)	$E_{6p}\ -\ E_{6s}$ (Exp.) [7]
$n = 7$	9199	10302	
$n = 8$	9200.44	10285	
$n = 9$	9200.69	10324.85	
$n = 10$	9201.48	10318.34	
$n = 11$	9201.16	10332.14	
$n = 12$	9201.27	10329.77	
$n = 13$	9201.09	10329.8	11177.84

4.1. Calculations of the hyperfine structure parameters

The hyperfine interaction is similar to the scalar-pseudoscalar symmetry breaking interaction in that they both arise from an interaction mainly localized at the nucleus. Accurate values for the hyperfine interaction constants thus give an indication that also the scalar-pseudoscalar matrix elements are reliable. Using the same models for the generation of CSFs for MCDHF

wave function expansions, as in the calculations of the energy, we computed the magnetic dipole constants A_J for the two atomic states $\left|6s\ ^2P_{1/2}\right\rangle$ and $\left|6p\ ^2P_{1/2}\right\rangle$ of ^{133}Cs. For ^{133}Cs, $I = 7/2$ and $\mu = 2.579$ nuclear magnetons. The results are shown in Table 2. The two models give values that are too small compared to experiment, and further improvements of the multiconfiguration expansion are needed before the values can compete with the highly accurate values from the MBPT calculations by Sahoo *et al.* [10].

Table 2 Calculated A_J constants for $\left|6s\ ^2P_{1/2}\right\rangle$ and $\left|6p\ ^2P_{1/2}\right\rangle$ of ^{133}Cs (in MHz) in the two models as functions of the active set.

AS	A_{6s} (1)	A_{6p} (1)	A_{6s} (2)	A_{6p} (2)	A_{6s} (Exp.) [8]	A_{6p} (Exp.) [8]
$n = 7$	1667.5	192.6	1721.5	195.6		
$n = 8$	1671.5	198.9	1703.6	198.7		
$n = 9$	1701.2	203.1	1725.3	200.2		
$n = 10$	1702.5	208.4	1732.3	205.8		
$n = 11$	1719.9	207.4	1749.6	204.6		
$n = 12$	1719.0	209.1	1746.8	206.8		
$n = 13$	1736.9	209.6	1746.8	206.5	2298.16	291.90

4.2. Calculations of the $S - PS$ interaction constant

Using MCDHF wave functions in the two models and the extended GRASP package, we calculated the $S - PS$ interaction and electric dipole matrix elements,

$$\langle S - PS\rangle \ = \ \sqrt{2}\ \frac{\left\langle\ \Psi(6s\ ^2S_{1/2}\ )\ \middle|\ \hat{H}_{S-PS}\ \middle|\ \Psi(6p\ ^2P_{1/2})\ \right\rangle}{C_{S-PS}\ G_F\ A} \tag{10}$$

$$\langle EDM\rangle \ = \ \left\langle\ \Psi(6s\ ^2S_{1/2})\ \middle|\ \hat{D}_Z\ \middle|\ \Psi(6p\ ^2P_{1/2})\ \right\rangle. \tag{11}$$

The results are presented in Table 3 (in a. u.).

Combining the matrix elements from Table 3 with the experimental limit [9] of the static electric dipole moment D_A of the ground state we obtain an upper limit for the constant C_{S-PS} (see Table 4). Calculated limits of C_{S-PS} are in good agreement with other theories [10].

Table 3 The values of EDM and S-PS interaction operator matrix elements in the two models as functions of the active set.

AS	$\langle EDM\rangle$ (1)	$\langle S - PS\rangle$ (1)	$\langle EDM\rangle$ (2)	$\langle S - PS\rangle$ (2)
$n = 7$	-2.137507	0.531368	-2.0690995	0.600011
$n = 8$	-2.135295	0.533322	-2.052946	0.606987
$n = 9$	-2.135780	0.534829	-2.055031	0.601420
$n = 10$	-2.134587	0.532404	-2.059800	0.604534
$n = 11$	-2.134851	0.532091	-2.060691	0.603568
$n = 12$	-2.134498	0.530297	-2.061189	0.601368
$n = 13$	-2.134686	0.529519	-2.061199	0.601272

Table 4 The values of the scalar - pseudoscalar interaction constant in the two models as a function of active set.

ASF	C_{S-PS} (1)	C_{S-PS} (2)	C_{S-PS} [9]
$n = 11$	3.00292×10^{-6}	3.07968×10^{-6}	
$n = 12$	3.01361×10^{-6}	3.08950×10^{-6}	
$n = 13$	3.01772×10^{-6}	3.08998×10^{-6}	2.24719×10^{-6}

5. Conclusions

The results obtained show that it is possible to investigate parity and time reversal symmetry violations in many-electron atoms using the MCDHF method. More accurate calculations can be carried out using orbitals optimized for the even and odd atomic states independently and calculating electric dipole and $S-PS$ interaction operator matrix elements with bi-orthonormal transformations [11]. The generalization of the MCDHF method presented in this work can also be used for investigations of the violations of the fundamental discrete symmetries induced by non-$(S - PS)$ interactions.

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