Computational modelling parity nonconservation and electroweak interaction effects in heavy atomic systems within the nuclear-relativistic many-body perturbation theory

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Computational modelling parity nonconservation and electroweak interaction effects in heavy atomic systems within the nuclear-relativistic many-body perturbation theory

O Yu Khetselius, A V Glushkov, M Yu Gurskaya, A A Kuznetsova, Yu V Dubrovskaya, I N Serga and L A Vitavetskaya

Odessa State Environmental University, L'vovskaya str.15, Odessa-16, 65016, Ukraine

E-mail: dirac13@mail.ru

Abstract. Computing the hyperfine coupling constants and parity non-conservation (PNC) effect parameters in a few heavy atomic systems has been performed and based on the combined relativistic nuclear mean-field theory and relativistic many-body perturbation theory (PT) formalism with accounting for the interelectron correlation and dominant QED corrections. Results of estimating hyperfine structure constants and PNC parameters for different heavy atoms (caesium, ion of barium, thallium, ytterbium) are presented and compared with other theoretical and experimental data. The spin-dependent contributions to the PNC amplitude for the caesium are presented too.

1. Introduction

Although the spectacular experimental achievements of particle physics in the last decade have strengthened the Standard Model (SM) as an adequate description of nature, they have also revealed that the SM matter represents a mere 5% or so of the energy density of the Universe, which clearly points to some physics beyond the SM despite the desperate lack of direct experimental evidence [1-6]. The sector responsible for the spontaneous breaking of the SM electroweak symmetry is likely to be the first to provide experimental hints for this new physics. The detailed review of these topics can be found in Refs. [1-6], in particular, speech is about brief introducing the SM physics and the conventional Higgs mechanism and a survey of recent ideas on how breaking electroweak symmetry dynamics can be explained. Further one could remind that the observation of a static electric dipole moment of a many-electron atom which violates parity, P , and time reversal, T , symmetry, represents a great fundamental interest in searching for a new physics beyond the SM of elementary particles [1-23]. The interaction mixes a parity of atomic states and also induces a static electric dipole moment of the atom. At the present time, different methods have been used in calculation of the hyperfine structure parameters, PNC and similar effects characteristics.

The most popular methods for computing the electron structure, hyperfine coupling constants, parity and time reversal symmetry violations parameters in heavy many-electron atoms are the multiconfiguration Dirac-Fock (MCDF) and relativistic cluster-coupled (RCC) methods. Besides there have been developed and intensively applied the different versions of a many-body relativistic and QED perturbation theory (PT), namely, the PT with the relativistic Hartree-Fock (RHF), the Dirac-Fock (DF), the Dirac-Kohn-Sham (DKS) zeroth approximations [6-23]. In order to provide a

consistent studying the hyperfine coupling constants, PNC effect parameters in the heavy atomic systems, these methods are combined with the different approaches to treat a nuclear structure and the corresponding nuclear effects such as the Bohr-Weisskopf and Breit-Rosenthal-Crawford-Schawlow effects, the skin neutron correction etc. Here the most popular approach is the relativistic mean-filed (RMF) model (see [24-27] and references there in) in different realizations. In Refs.[28-33] we have presented our version of the relativistic PT with an optimized DKS zeroth approximation and correct accounting for the interelectron correlations and dominant QED corrections, combined with the RMF nuclear model (N-QED). In present paper this approach is used for computing the hyperfine structure constants, electroweak interaction and PNC effect parameters in the heavy atomic systems. The N-QED approach allows to fulfil studying the spectra of the multi-electron atomic systems with the correct account of the relativistic, interelectron correlation, nuclear, radiative effects [33-45]. All interelectron correlation corrections of the second order and dominated classes of the higher orders diagrams have been taken into account. Results of estimating these constants for different heavy atoms (caesium, ion of barium, thallium, ytterbium) are presented and compared with other theoretical and experimental data. The spin-dependent contributions to the parity PNC amplitude are presented too.

2. Nuclear-relativistic perturbation theory approach to hyperfine, electroweak effects in heavy atoms

The main elements of the relativistic PT formalism with the optimized DKS zeroth approximation and correct accounting for the interelectron correlations and dominant QED corrections, combined with the RMF nuclear model, are in details presented in Refs. [24-40]. Here we are limited only by the key elements. The relativistic PT zeroth approximation electron wave functions are found from the Dirac equation solution with a self-consistent potential, which includes the core ab initio DKS potential, electric, polarization potentials of a nucleus. All correlation corrections of the second and high orders of PT (electrons screening, particle-hole interaction etc.) are accounted for [24-28].

The nuclear model is based on the relativistic mean-field (RMF) model, which is usually designed as a renormalizable meson-field theory for nuclear matter and finite nuclei (see details in [23-28]). Its relatively successful application in nuclear calculations is usually explained by the fact that the RMF model can incorporate certain ground-state correlations and yields a ground-state description beyond the literal mean-field picture [25]. In our computing there is used NL3-NLC scheme, which is among the most successful parameterizations available. As it is indicated in Ref.[25], the strong attractive scalar (*S:* -400 MeV) and repulsive vector (*V:* +350 MeV) fields provide both the binding mechanism (*S* + *V:* -50 MeV) and the strong spin-orbit force (*S* – *V:* -750 MeV) of both right sign and magnitude.

In order to compute radiation transition amplitudes we have used an advanced gauge-invariant version of the generalized relativistic energy approach (see details in Refs. [11,32,36]). Simultaneously, this theory provides powerful ab initio method of construction of the optimized PT basis and consistent treating gauge-dependent multielectron contributions $\mathrm{Im}\Delta E_{\mathrm{ninv}}$ of the lowest relativistic PT corrections to the atomic level radiation width. This value is considered to be the typical representative of the multielectron exchange-correlation effects contributions. The method used allows to estimate an effectiveness of accounting for the multielectron exchange-correlation effects and provides the practical way of the refinement of the atomic characteristics calculations, based on the "first principles".

Let us consider the key elements of the scheme of calculating the PNC transition amplitude. The dominative contribution to the PNC amplitude is provided by the spin-independent part of the operator of the weak interaction, which should be added to the standard atomic Hamiltonian [2,6]:

$$H = H_{at} + \mu \sum_j H_W(j), \tag{1}$$

$$H_W^1 = \frac{G}{2\sqrt{2}} Q_W \gamma_5 \rho(r), \tag{2}$$

where G_F is the Fermi constant of the weak interaction, γ_5 is the Dirac matrice, $\rho(r)$ is a density of the charge distribution in a nucleus and Q_W is a weak charge of a nucleus, linked with number of neutrons N and protons Z and the Weinberg angle θ_W in the Standard model (c.f. [1-3]) as:

$$Q_W = Z(1-4\sin^2\theta_W) - N \tag{3}$$

With account for the radiative corrections, equation (3) can be rewritten as [2]:

$$Q_W = \{Z(1-[4.012 \pm 0.010]\sin^2\theta_W) - N\}\cdot(0.9857 \pm 0.0004)(1+0.0078\,T)$$
$$\sin^2\theta_W = 0.2323 + 0.00365\,S - 0.00261\,T) \tag{4}$$

The parameters S,T parameterize the looped corrections in the terms of conservation (S) and violation (T) of an isospin. As it is known, the spin-dependent contribution to the PNC amplitude has three distinct sources: a nuclear anapole moment (it is usually considered as an electromagnetic characteristics of system, where the PNC takes a place; generally speaking, speech is about an emerged spin structure and the magnetic field distribution is similar to the solenoid field), the *Z*-boson exchange interaction from nucleon axial-vector currents (A_nV_e), and the combined action of the hyperfine interaction and spin-independent *Z*-boson exchange from nucleon vector (V_nA_e) currents [2,6,7]. The anapole moment contribution strongly dominates. The above-mentioned interactions can be presented by the following Hamiltonian

$$H_W^i = \frac{G}{\sqrt{2}} k_i (\alpha \cdot I)\rho(r) \tag{5}$$

where $k(i$=a) is an anapole contribution, $k(i$=2)=k_{Z0} is axial-vector contribution, $k(i$=kh)=k_{Qw} is a contribution due to the combined action of the hyperfine interaction and spin-independent Z exchange one. Calculation of the corresponding matrix elements is reduced to the computing the integrals as follows [6,15]:

$$< i \mid H_W^1 \mid j >= i\frac{G}{2\sqrt{2}} Q_W \delta_{k_i - k_j}\delta_{m_i m_j}\int_0^\infty dr[F_i(r)G_j(r) - G_i(r)F_j(r)]\rho(r) \tag{6}$$

The reduced matrix element can be written as:

$$< i \parallel H_W^1 \parallel j >= i\frac{G}{2\sqrt{2}} Q_W \int_0^\infty dr[F_i(r)G_j(r) - G_i(r)F_j(r)]\rho(r) \tag{7}$$

Further the general expression for the corresponding PNC amplitude for the *a*-*b* transition is written as follows:

$$< a \mid PNC \mid b >= -\sum_n [\frac{< b \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid a >}{\varepsilon_a - \varepsilon_n} + \frac{< b \mid H_W^{(1)} \mid n >< n \mid e\alpha_\nu A^\nu \mid a >}{\varepsilon_b - \varepsilon_n} \tag{8}$$

The corresponding spin-dependent PNC contribution is :

$$< a \mid PNC \mid b >^{sd} = k_a < a \mid PNC \mid b >^{(a)} + k_2 < a \mid PNC \mid b >^{(2)} + k_{hf} < a \mid PNC \mid b >^{(hf)} \tag{9}$$

where

$$< a \mid PNC \mid b >^{(hf)} =$$

$$= \sum_{\substack{m\neq a\\ n\neq a}} \frac{< a \mid H_W^{(1)} \mid n >< n \mid H_W^{(hf)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_a - \varepsilon_n)} + \sum_{\substack{m\neq a\\ n\neq a}} \frac{< a \mid H_W^{(hf)} \mid n >< n \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_a - \varepsilon_n)} +$$

$$+ \sum_{\substack{m\neq a\\ n\neq b}} \frac{< a \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid m >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} + \sum_{\substack{m\neq a\\ n\neq b}} \frac{< a \mid H_W^{(hf)} \mid m >< m \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} +$$

$$+ \sum_{\substack{m\neq b\\ n\neq b}} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid m >< m \mid H_W^{(hf)} \mid b >}{(\varepsilon_b - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} + \sum_{\substack{m\neq b\\ n\neq b}} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid m >< m \mid H_W^{(1)} \mid b >}{(\varepsilon_b - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} -$$

$$- < a \mid H_W^{(hf)} \mid a > \sum_{m\neq a} \frac{< a \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)^2} - \sum_{n\neq b} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid b >}{(\varepsilon_b - \varepsilon_n)^2} < b \mid H_W^{(hf)} \mid b > . \quad (10)$$

Here the following notations are used: $\mid a >= \mid aIF_F M_F >$, $\mid b >= \mid bIF_I M_I >$, I – spin of a nucleus, $F_{I,F}$-is a total momentum of an atom and M – its z component (I,F are the initial and final states). It should be noted the expressions for the matrix elements $< a \mid PNC \mid b >^{(a)}$, $< a \mid PNC \mid b >^{(2)}$are similar to equation (6). The detailed description of the corresponding matrix elements, procedures of their computing and other aspects of the general method and PC code is presented in Refs.[28-45].

3. Results and conclusions

Here we present the results of computing the hyperfine structure parameters for the neutral caesium and Cs-like ion of barium Ba^+. In Table 1 the experimental (A^{Exp}) and our ($A^{N\text{-}Qed}$) data for magnetic dipole constant A (MHz) for the valent states of ^{133}Cs ($I=7/2$, $g_i=0.7377208$) are presented. The calculation results, obtained within the standard (A^{RHF}) RHF and RHF with account of the second and higher PT corrections, the MCDF approximation and QED formalism [22,23] are listed too. In a whole there is a physically reasonable agreement of our data with experimental ones that is provided by using the gauge-invariant relativistic orbital basis and the correct accounting for the exchange-correlation, nuclear, QED effects.

Table 1. The values (MHZ) of the hyperfine structure constant A for valent states of ^{133}Cs: A^{Exp} - experiment; A^{RHF}, dA^{RHF} - RHF calculation plus the second and higher PT orders contribution; A^{QED} – data [17,18]; $A^{N\text{-}Qed}$ – the present paper;

State	A^{MCDF}	A^{RHF}	$A^{RHF}+dA$	A^{Qed}	$A^{N\text{-}Qed}$	A^{Exp}
$6s_{1/2}$	1736.9	1426.81	2291.00	2294.45	2296.85	2298.16
$6p_{1/2}$	209.6	161.09	292.67	292.102	291.97	291.90(13)

In Table 2 we present the results of calculating the hyperfine structure constant A for different states of the Cs-like ion of barium: $[5p^6]6s_{1/2},6p_{1/2}$. The following notations are used: A^{RCC} – results of calculation on the basis of the RCC method; A^{DF} – DF method; A^{RHF} - RHF method and A^{QED}- the QED calculation (from Refs. [13-23]); $A^{N\text{-}Qed}$ – our results.

Table 2. Theoretical and experimental data for the hyperfine structure constant A for the states of the Cs-like ion Ba (see text)

State	A^{Exp}	A^{RCC}	A^{DF}	A^{RHF}	A^{QED}	$A^{\text{N-Qed}}$
$[5p^6]6s_{1/2}$	4018	4072.83	4193.02	4208.2	4014.52	4016.76
$[5p^6]6p_{1/2}$	742.04	736.98	783.335	---	742.96	742.54

Further in Table 3 we list the nuclear spin dependent corrections to the PNC ^{133}Cs 6s-7s amplitude E_{PNC}, calculated by different theoretical methods (in units of the $k_{a,2,hf}$ coefficient): many-body PT (MBPT), DF-PT, the shell model, N-QED PT (present paper) (from Refs. [7-20]). In Table 4 there are presented the theoretical values of the weak charge Q_W for three heavy atoms, predicted in the Standard Model and different approaches (from Refs. [6-9]).

Table 3. The nuclear spin-dependent corrections to the PNC ^{133}Cs: 6s-7s amplitude E_{PNC}, calculated by different methods (in units of $k_{a,2,hf}$ coeff.): MBPT, DF-PT, shell model, N-QED PT (see text).

Correction	MBPT	Shell model	DF	This work
K (sum)	0.1169	0.1118	0.112	0.1159
k_2- the Z-boson exchange interaction from nucleon axial-vector currents (A_nV_e)	0.0140	0.0140	0.0111 0.0084	0.0138
k_{hf} - the combined action of the hyperfine interaction and spin-independent Z exchange	0.0049	0.0078	0.0071 0.0078	0.0067
k_a –anapole moment	0.0980	0.090	0.0920	0.0954

Table 4. The estimated values of the weak charge Q_W for heavy atoms, predicted in different approaches (see text)

Atom:	Standard Model	RHF+Breit	MCDF	MBPT	This work
^{133}Cs	-73.19(3)	-72.66	-69.78	-72.69	-72.62
		-71.70	-71.09	-72.18	
^{173}Yb	-96.85(6)	-	-	-	-95.41
^{205}Tl	-116.81(4)	-116.20	-	-	-116.15

The key requirements to the precise computing PNC amplitudes are connected with the correct accounting for the inter electron correlations, relativistic, Breit and radiative and nuclear corrections (including the Bohr-Weisskopf and Breit-Rosenthal-Crawford-Schawlow effects, i.e. a magnetic moment distribution in a nucleus, the skin neutron and other corrections). The analysis of results shows that in principle a majority of theoretical approaches provides physically reasonable agreement with the SM data, but the important question is how much exact this agreement. The theoretical data on the constants directly indicate the necessity of new, more precise experiments. From the other side, it is of a great interest to study the PNC effect in other heavy atoms such lanthanides and actinides atoms. The rare-earth elements are especially interesting as they have very complicated spectra of autoionization resonances (with very unusual their behavior in a weak electric and laser fields from physical viewpoint [35]). The elementary analysis shows that the perspectives of the PNC experiments with Stark pumping of the individual states in the rare-earth and other heavy atoms (and probably more effective multicharged ions of these elements) and simultaneously polarized laser field dressing (with a cold-atom fountain or interferometer) could provide comfortable conditions for precise observation of the electroweak effects.

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