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SENSING NUCLEAR ANAPOLE MOMENT AND PARITY NON-CONSERVATION EFFECT IN HEAVY ATOMIC SYSTEMS: NEW SCHEME

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Abstract. It is presented the new theoretical approach for sensing anapole moment of a nucleus and parity non-conservation effect in heavy atomic systems, based on the combined QED perturbation theory formalism and relativistic nuclear mean-field theory. Results of estimating these constants are presented.
Keywords: anapole moment, parity non-conservation, heavy atomic systems

О ДЕТЕКТРОВАНИИ АНАПОЛЬНОГО МОМЕНТА ЯДРА И ЭФФЕКТА НЕСОХРАНЕНИЯ ЧЕТНОСТИ В ТЯЖЕЛЫХ АТОМНЫХ СИСТЕМАХ: НОВЫЙ ПОДХОД

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Аннотация. Представлен новый теоретический подход к детектированию анапольного момента ядра и эффекта несохранения четности в тяжелых атомных системах, базирующийся на ядерно-КЭД теории возмущений и релятивистской ядерной модели среднего поля. Приведены результаты расчета искомых параметров.
Ключевые слова: анапольный момент, несохранение четности, тяжелые атомные системы

ПРО ДЕТЕКТУВАННЯ АНАПОЛЬНОГО МОМЕНТУ ЯДРА ТА ЕФЕКТУ НЕЗБЕРЕЖЕННЯ ПАРНОСТІ У ВАЖКИХ АТОМНИХ СИСТЕМАХ: НОВИЙ ПІДХІД

О. Ю. Хецеліус

Анотація. Розглянутий новий теоретичний підхід до детектування анапольного моменту ядра та ефекту незбереження парності у важких атомних системах, який базується на ядерно-КЕД теорії збурень та релятивістській моделі середнього поля. Наведені результати розрахунку шуканих параметрів.

Ключові слова: анапольний момент, незбереження парності, важкі атомні системи

1. Introduction

At present time a great attention is turned on development of the effective nuclear schemes and technologies for sensing different nuclear properties, creation of the corresponding nuclear sensors. In fact speech is about a new branch in the modern nuclear and sensors science. From the other side, it gives a new pulse for further developing a modern as atomic and as nuclear theories too. Studying the spectral lines hyperfine structure (hfs) for heavy elements and ions, sensing an anapole moment and corresponding spin-dependent parity non-conservation (PNC) effect in heavy atomic systems are the most actual and complicated topics of modern theory [1-11]. Naturally, from the theoretical point of view, the well-known multi-configuration relativistic Hartree-Fock (RHF) and Dirac-Fock (MCDF) approaches are the most reliable version of calculation for heavy multi-electron atomic systems with a large nuclear charge (look [12,13]). As a rule, the one- and two-particle relativistic effects are taken in these calculations into account practically precisely. The next important step is an adequate account for the nuclear and QED corrections. This topic has been a subject of intensive theoretical and experimental interest (see [1-11]). It is well known that the the parity nonconservation experiments in atomic physics provide an important possibility to deduce information on the Standard Model independent of the known high-energy experiments [1]. The detailed review of these topics can be found in refs.[1-9], where one could find a brief introducing the Standard Model 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 Standard model of particles. In the present paper the new theoretical approach is used for sensing the hyperfine structure parameters, anapole moment of a nucleus and PNC effect in heavy atomic systems.

2. Nuclear-QED PT approach to sensing hyperfine structure parameters and parity-non-conservation transition amplitude

As the basis of our approach it is used the nuclear-QED perturbation theory (PT) which is the combining ab initio QED PT formalism and nuclear relativistic middle-field (RMF) model [14-20]. The important feature is the correct accounting for the inter electron correlations, nuclear, Breit and QED corrections. The wave electron functions zeroth basis is found from the Dirac equation solution with potential, which includes the core ab initio potential $V(r|SCF)$, electric $V(r|nlj)$, polarization $V_{pol}(r|nlj)$+potentials of nucleus. All correlation corrections of the second and high orders of PT (electrons screening, particle-hole interaction etc.) are accounted for [10]. The concrete nuclear model is based on the relativistic mean-field (RMF) model for the ground-state calculation of the nucleus. In our approach we have used so called NL3-NLC and generalized Ivanov et al approach (see details in refs. [5,19,20]), which are among the most successful parameterizations available. Further one can write the Dirac-Fock -like equations for a multi-electron system {core-*nl*j}. Formally they fall into one-electron Dirac equations for the orbitals *nlj* with potential: $V(r)=V(r|SCF)+V(r|nl\ j)+V(r|R)+V_{ex}+V_c$. Radial parts *F* and *G* of two components of the Dirac function for electron, which moves in the potential *V(r,R)* are defined by solution of the Dirac equations (PT zeroth order). The terms V_{ex} and V_c of the general potential accounts for exchange and correlation inter-electron interaction. The exchange effects are accounted for in the first two PT orders. The core electron density is defined by iteration algorithm within QED procedure [13-15]. The radiative QED (the self-energy part of the Lamb shift and the vacuum polarization contribution) are accounted for within the QED formalism [5,13-15]. The hyperfine structure constants are defined as follows. The interaction Hamiltonian has the standard form:

$$H_I = e\overline{j}_e^{\mu}\overline{A}_{\mu} + e\overline{J}_N^{\mu}\overline{A}_{\mu}, \qquad (1)$$

where j_e^{μ}, j_N^{μ} are Lorentz covariant current operators for the electron and the nucleus:

$$\overline{j}_e^{\mu} = \hat{\overline{\psi}}_e \gamma^{\mu} \hat{\psi}_e, \qquad (2)$$

$$\overline{J}_N^{\mu} = \frac{1+\tau_3}{2}\hat{\overline{\psi}}_N \gamma^{\mu} \overline{\psi}_N + \frac{\lambda}{2M}\partial_{\nu}(\hat{\overline{\psi}}_N \sigma^{\mu\nu} \overline{\psi}_N). \qquad (3)$$

Here $\sigma^{\mu\nu} = \frac{1}{2}\left[\gamma^{\mu}, \gamma^{\nu}\right]$. The rest notations are standard. Using the first-order perturbation based on the S-matrix method one can get the expression for the hyperfine structure parameters [16]. As usually, the corresponding reduced matrix element can be divided on the electron part and on the Dirac part and the anomalous part for a nucleus. In order to define all parts the corresponding relativistic wave functions of the electron and single-particle states of a nucleus are required.

The dominative contribution to the PNC amplitude is provided by the spin-independent part of the operator for a weak interaction:

$$H_W^1 = \frac{G}{2\sqrt{2}} Q_W \gamma_5 \rho(r), \qquad (4)$$

where $G_F = g^2/4\sqrt{2}m_W^2$ is the Fermi constant of the weak interaction, γ_5 –is the Dirac matrice, *ρ(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:

$$Q_W = Z(1 - 4\sin^2\theta_W) - N. \qquad (5)$$

With account for the radiative corrections, equation (5) can be rewritten as [5,18]:

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

$$\sin^2\theta_W = 0.2323 + 0.00365S - 0.00261T). \qquad (6)$$

The parameters S,T parameterize the looped corrections in the terms of conservation (S) and violation (T) of an isospin.

The spin-dependent contribution to the PNC amplitude has three distinct sources: the nuclear anapole moment, 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 (look, for example, [3-8]. As a rule, the anapole moment contribution strongly dominates. From physical point of view, anapole moment can be considered as an electromagnetic characteristics of system, where the PNC takes a place; generally speaking, speech is about the arisen spin structure and the magnetic field distribution is similar to the solenoid field. The above-mentioned interactions can be represented by the Hamiltonian

$$H_W^i = \frac{G}{\sqrt{2}} k_i (\alpha \cdot I)\rho(r), \qquad (7)$$

where k(i=a) is an anapole contribution, k(i=2)=k_{Z0} - 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 . The estimate of the corresponding matrix elements is in fact reduced to the calculation of the integrals as:

$$< i \mid H_W^1 \mid j >= i\frac{G}{2\sqrt{2}} Q_W \delta_{k_i - k_j} \delta_{m_i m_j} \times$$
$$\times \int_0^\infty dr[F_i(r)G_j(r) - G_i(r)F_j(r)]\rho(r). \quad (8)$$

The reduced matrix element has the standard form as follows:

$$< i \parallel H_W^1 \parallel j >= i\frac{G}{2\sqrt{2}} Q_W \int_0^\infty dr[F_i(r)G_j(r) - \quad (9)$$
$$- G_i(r)F_j(r)]\rho(r).$$

The general expression for the corresponding spin-dependent PNC contribution is:

$$< a \mid PNC \mid b >^{sd} = k_a < a \mid PNC \mid b >^{(a)} + k_2$$
$$< a \mid PNC \mid b >^{(2)} + k_{hf} < a \mid PNC \mid b >^{(hf)}, \quad (10)$$

where, for example, the element looks as follows:

3. Results and conclusions

As the first studying objects, we have considered the nuclei of isotopes of ^{133}Cs and Cs-like ion of barium. We carried out calculation (the Superatom-ISAN and RMF-G package [13-15,20] are used) the hyperfine structure (hfs) parameter for Cs and Ba^+ isotopes. In table 1 the experimental (A^{Exp}) and our ($A^{N\text{-}Qed}$) data for magnetic dipole constant A (MHz) for valent states of ^{133}Cs (*I=7/2*, $g_i=0.7377208$) and the Cs-like ion of barium: [5p^6]6s$_{1/2}$,6p$_{1/2}$ are presented. The following notations are used: A^{DF} – MCDF method ; A^{RHF} - RHF method and A^{QED}- the QED theory; $A^{N\text{-}Qed}$ is the result of the present paper (from refs. [5,8,9,10,16]. In a whole the key quantitative factor of agreement between the theory and experimental data is connected with using the gauge-invariant relativistic orbital basis's, the correct accounting for the inter electron correlations, nuclear, Breit, QED radiative corrections (including magnetic moment distribution in a nucleus and nuclear corrections).

$$< a \mid PNC \mid b >^{(hf)} =$$
$$\sum_{\substack{m\neq a\\ n\neq a}} \frac{< a \mid H_W^{(1)} \mid n >< n \mid H_W^{(hf)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_a - \varepsilon_n)} + \sum_{\substack{m\neq a\\ n\neq a}} \frac{< a \mid H_W^{(hf)} \mid n >< n \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_a - \varepsilon_n)} +$$
$$+ \sum_{\substack{m\neq a\\ n\neq b}} \frac{< a \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid m >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} + \sum_{\substack{m\neq a\\ n\neq b}} \frac{< a \mid H_W^{(hf)} \mid m >< m \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid b >}{(\varepsilon_a - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} +$$
$$+ \sum_{\substack{m\neq b\\ n\neq b}} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid m >< m \mid H_W^{(hf)} \mid b >}{(\varepsilon_b - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} + \sum_{\substack{m\neq b\\ n\neq b}} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(hf)} \mid m >< m \mid H_W^{(1)} \mid b >}{(\varepsilon_b - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} - \quad (11)$$
$$- < a \mid H_W^{(hf)} \mid a > \sum_{m\neq a} \frac{< a \mid H_W^{(1)} \mid m >< m \mid e\alpha_\nu A^\nu \mid b >}{(\varepsilon_a - \varepsilon_m)^2} - \sum_{n\neq b} \frac{< a \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid b >}{(\varepsilon_b - \varepsilon_n)^2} < b \mid H_W^{(hf)} \mid b >.$$

Here the following notations are used: $| a >=| aIF_F M_F >, | b >=| bIF_I M_I >$, *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 (14).

Table 1**.** The values (MHZ) of the hfs constant A for valent states of ^{133}Cs and the Cs-like ion of Ba: A^{Exp} - experiment; A^{RHF}, dA^{RHF} - RHF calculation plus the second and higher PT orders contribution; A^{QED} – QED theory [32]; $A^{N\text{-}Qed}$ – the present paper;

	State	A^{MCDF}	A^{RHF}	$A^{RHF}+dA$	A^{Qed}	$A^{N\text{-}Qed}$	A^{Exp}
Cs	$6s_{1/2}$	1736,9	1426,81	2291,00	2294,45	2296,85	2298,16
Cs	$6p_{1/2}$	209,6	161,09	292,67	292,102	291,97	291,90(13)
Ba^+	$6s_{1/2}$	4193,02	4208,2	2291,00	4014,52	4016,76	4018
Ba^+	$6p_{1/2}$	783,335	---	292,67	742,96	742,54	742,04

Further in table 2 we present new data on 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 nuclear shell model and our approach [5-8].

Table 2. The nuclear spin-dependent corrections to PNC ^{133}Cs: 6s-7s amplitude, 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	Our data
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

Analysis shows that the many-body theories provide the maximal value of the nuclear spin-dependent contribution to the PNC 6s-7s amplitude in ^{133}Cs, at the same time purely nuclear estimates give a minimal value of this parameter. Let us also remind that as a rule the presented theoretical approaches provides physically reasonable agreement with the data of Standard Model, but the important question is how much exact this agreement. In our opinion, the précised estimates within the N-QED theory indicate on the tiny deviation from the Standard model. Summering all above said, let us conclude that a new effective theoretical approach for sensing hyperfine structure parameters, anapole moment and PNC effect parameters in heavy atomic systems is presented and based on the combined QED perturbation theory formalism and relativistic nuclear mean-field theory. The concrete sensing the anapole moment and PNC parameters confirms its adequacy and theoretical consistence. We believe that a new approach can be usefully applied in sensing the corresponding parameters for more complicated systems than the cesium.

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