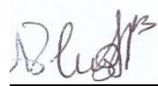


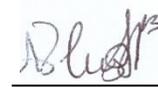
МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

**Methodical instructions
for practical work, test performance,
distance learning of PhD students
in the discipline “OPTICS AND SPECTROSCOPY OF
RELATIVISTIC ATOMS AND MULTIPLE-CHARGED IONS”, Part 3
(Training of PhD students of the specialty: 104 –
“Physics and Astronomy” and others)**

«Затверджено»
на засіданні групи забезпечення спеціальності
Протокол №4 від 13/05/2023
Голова групи забезпечення


проф. Глушков О.В.

«Затверджено»
на засіданні кафедри вищої та прикладної математики
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Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline “OPTICS AND SPECTROSCOPY OF RELATIVISTIC ATOMS AND MULTIPLE-CHARGED IONS”, Part 3. (Training specialty: 104 - “Physics and Astronomy” and others)

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PREFACE

Discipline " OPTICS AND SPECTROSCOPY OF RELATIVISTIC ATOMS AND MULTIPLE-CHARGED IONS " is an elective discipline in the cycle of professional training of postgraduate or PhD students (third level of education) in the specialty 104- Physics and Astronomys.

It is aimed at: i) K11 Ability to analyze and identify a complex of major problems in a certain field of modern physics and, in particular, optics and spectroscopy of atoms, multi-charged ions, molecular, quantum, laser systems, solids, as well as the atmosphere and ocean; Ability to develop new and improve existing methods of describing optical and spectroscopic properties of solids based on methods of quantum mechanics, quantum chemistry of solids, as well as methods of relativistic quantum theory; ii). K12 The ability to create physical, mathematical and computer models in optics and spectroscopy of physical systems with the implementation of effective algorithms and specialized software. Ability to acquire new fundamental knowledge in optics and spectroscopy of atoms, molecules, solids, laser systems, as well as geophysical systems (atmosphere and ocean). These methodical instructions are for self-studying work of the second-year PhD students and tests performance in the discipline "Quantum Geometry and Dynamics of Resonances".

Program learning outcomes include: P111 Ability to conduct research on optics and spectroscopy of atoms, multi-charged ions, molecular, quantum, laser systems, solid bodies, as well as the atmosphere and ocean in the context of existing theories, make reasoned conclusions (including assessment of the degree of uncertainty) and proposals for further research; P112 The ability to use modern or develop new approaches to the calculation of fundamental characteristics, in particular, based on methods of quantum mechanics, electrodynamics, electronics in optics and spectroscopy of atoms, molecules, solids, laser systems, as well as geophysical systems (atmosphere and ocean); P121 The ability to create physical, mathematical and computer models in the optics and spectroscopy of atoms, molecules, solids, laser systems, solids, as well as geophysical systems (atmosphere and ocean), check ix adequacy, research ix to obtain new conclusions and deepen understanding of fundamental processes in the physical system, analyzing limitations; P122 The ability to achieve relevant knowledge using effective, including new methods, models, algorithms for determining the physical (optical and spectroscopic) characteristics of atoms, molecules, solids, laser systems, as well as geophysical systems (atmosphere and ocean), processing the results of numerical and natural experiments.

The main topic of this work is a Resonance dynamics for quantum systems in an electromagnetic field. Methods for calculating energies and widths of Stark resonances (Look Syllabus of the discipline, edition 2023)

I. Topic: Hyperfine and electroweak interaction in heavy finite Fermi systems and the effect of non-conservation of parity (L2.7) (L 2.7)

Торіс: Надтонка та електрослабка взаємодія у важких кінцевих фермі-системах та ефект незбереження парності (Л2.7)

1 Introduction

The parity non-conservation (PNC) or violation experiments in atomic physics provide an important possibility to deduce information on the Standard Model independent of high-energy physics experiments [1-40].

The recent LEP experiments are fulfilled [1,2], that yield extremely accurate values for Z-boson properties. In the last two decades a status of the Standard model has been strengthened by different experimental achievements of particle physics. It should be mentioned Higgs boson discovery, measurement of CP violations in the K^0 , B^0 mesons, evidence of accelerated expansion of the universe, determination of the fraction of dark energy and dark matter in the universe, etc. From the other side, there are a number of the serious factors which clearly points to some new physics beyond the Standard model despite the desperate lack of direct experimental evidence. One could remind that the density of matter included into the Standard model is approximately 5% of the energy density of the universe; besides, neutrinos in the Standard model are massless, and there are no neutrino oscillations (not to mention gravity). As it is known, the Standard model can be divided into three sectors: the calibration sector, the fragrance sector, and the symmetry-breaking sector. While the first two sectors are being actively studied in accelerator experiments (LEP, SLD, BELLE, etc.), the sector of spontaneous symmetry breaking is now attracting close attention, as it may give clear hints of existence in New Physics experiments beyond the Standard model.

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 a search of these hints. The detailed review of these topics can be found in Refs. [1-91].

Atomic optical and Stark pumping PNC measurements have been fulfilled in a whole number of heavy atoms, namely, in caesium (0.35 % accuracy [1]), thallium (1.7 %), bismuth (2 %), Pb (1.2 %) etc. The atomic optical tests of the Standard model provide important constraints on possible extensions of the SM. A recent analysis [2] of parity-violating electron-nucleus scattering measurements combined with atomic PNC measurements placed tight constraints on the weak neutral-current lepton-quark interactions at low energy, improving the lower bound on the scale of relevant new physics to \sim TeV. The precise measurement of the PNC amplitudes in Cs [1] led to an experimental

value of the small contribution from the nuclear-spin dependent PNC accurate to 14%. So, from the one side there is very actual necessity of the further development and increasing of the theoretical approaches accuracy and carrying out new atomic optical and Stark pumping PNC experiments.

The different methods have been used in calculation of the hyperfine structure parameters, PNC effect. The most popular multiconfiguration Dirac-Fock (MCDF) method for calculating parity and time reversal symmetry violations in many-electron atoms is often, however its application requires some additional generalizations [3,17,26]. Among other well-known calculation methods, a relativistic many-body perturbation theory (RMBPT), namely, the PT with relativistic Hartree-Fock (RHF) and Dirac-Fock (DF) zeroth approximations, the relativistic all-order method, QED perturbation theory (PT) etc should be mentioned (e.g.[9-70]).

In present paper we present the results of application of the consistent theoretical approach, namely, the nuclear-relativistic many-body perturbation theory (N-RMBPT), to study the hyperfine and electroweak interaction parameters in the heavy finite Fermi-systems and PNC effect. The N-RMBPT formalism is based on the combining ab initio perturbation theory formalism for electron subsystem, nuclear relativistic middle-field model for nuclear subsystem and an energy approach for computing radiation transition amplitude. It allows to fulfil computing the PNC amplitudes in the finite Fermi-systems (atomic systems) [3,10,41,42,49-54,92-101]. The important feature is the correct accounting for the inter electron correlations, nuclear, Breit and QED radiative corrections. All correlation corrections of the second order and dominated classes of the higher orders diagrams are taken into account. The results of calculation of the hyperfine structure parameters, the PNC amplitudes, the nuclear spin dependent corrections to the PNC, a weak charge Q_W for different atomic systems are presented and compared with available data in the literature.

2. Relativistic nuclear-RMBPT formalism in theory of heavy finite Fermi-systems

Here we present a brief description of the key moments of our approach (more details can be found in refs. [3,4,10, 64-98]). The wave electron functions zeroth basis is found from the Dirac equation solution with potential, which includes the self-consistent ab initio potential (in the Dirac-Kohn-Sham approximation), 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.

The concrete model for nuclear subsystem is based on the relativistic mean-field model for the ground-state calculation of the nucleus, which was developed as a renormalizable meson-field theory for nuclear matter and finite nuclei. The

realization of nonlinear self-interactions of the scalar meson led to a quantitative description of nuclear ground states. As a self-consistent mean-field model (for a comprehensive review see ref. [37,101]), its ansatz is a Lagrangian or Hamiltonian that incorporates the effective, in-medium nucleon-nucleon interaction. As a Kohn-Sham scheme, the relativistic mean-field model can incorporate certain ground-state correlations and yields a ground-state description beyond the literal mean-field picture. As indicated in Refs. [37,38] 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 our opinion, the most preferable one for the class of problems under consideration is so called NL3-NLC version (see details in refs. [3,61,69]), which are among the most successful parameterizations available.

Let us consider the procedure of computing the PNC transition amplitude. The dominative contribution to the PNC amplitude is provided by the spin-independent part of the operator for a weak interaction, which should be added to the atomic Hamiltonian [3]:

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

$$H_w^1 = \frac{G}{2\sqrt{2}} Q_w \gamma_5 \rho(r). \quad (2)$$

Here $G_F = g^2 / 4\sqrt{2}m_w^2$ is the Fermi constant of the weak interaction, γ_5 –is the Dirac matrix, $\rho(r)$ 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. [2,5]):

$$Q_w = Z(1 - 4\sin^2 \theta_w) - N \quad (3)$$

with accounting for the radiative corrections, equation (2) can be rewritten as [1,2]:

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

$$\sin^2 \theta_w = 0.2323 + 0.00365S - 0.00261T \quad (4)$$

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 a few distinct sources: the nuclear anapole moment ((that is 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 Z -boson exchange interaction from nucleon axial-vector currents ($A_n V_e$), and the combined action of the hyperfine interaction and spin-independent Z -boson exchange from nucleon vector ($V_n A_e$) currents (e.g.[3,10,28])

The above-mentioned interactions can be represented by the Hamiltonian

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

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. It is well known that the contribution into a PNC amplitude, provided by the anapole moment term, significantly dominates.

The estimate of the corresponding matrix elements is in fact reduced to the calculation of the following integrals [10]:

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

The reduced matrix element is as follows:

$$\langle i || H_W^1 || j \rangle = i \frac{G}{2\sqrt{2}} Q_W \int_0^\infty dr [F_i(r) G_j(r) - G_i(r) F_j(r)] \rho(r) \quad (7)$$

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

$$\langle a | PNC | b \rangle = - \sum_n \left[\frac{\langle b | e \alpha_v A^v | n \rangle \langle n | H_W^{(1)} | a \rangle}{\varepsilon_a - \varepsilon_n} + \frac{\langle b | H_W^{(1)} | n \rangle \langle n | e \alpha_v A^v | a \rangle}{\varepsilon_b - \varepsilon_n} \right] \quad (8)$$

The corresponding spin-dependent PNC contribution is:

$$\langle a | PNC | b \rangle^{sd} = k_a \langle a | PNC | b \rangle^{(a)} + k_2 \langle a | PNC | b \rangle^{(2)} + k_{hf} \langle a | PNC | b \rangle^{(hf)}, \quad (9)$$

where

$$\langle a | PNC | b \rangle^{(hf)} =$$

$$\begin{aligned}
& \sum_{\substack{m \neq a \\ n \neq a}} \frac{\langle a | H_W^{(1)} | n \rangle \langle n | H_W^{(hf)} | m \rangle \langle m | e\alpha_v A^v | b \rangle}{(\varepsilon_a - \varepsilon_m)(\varepsilon_a - \varepsilon_n)} + \sum_{\substack{m \neq a \\ n \neq a}} \frac{\langle a | H_W^{(hf)} | n \rangle \langle n | H_W^{(1)} | m \rangle \langle m | e\alpha_v A^v | b \rangle}{(\varepsilon_a - \varepsilon_m)(\varepsilon_a - \varepsilon_n)} \\
& + \sum_{\substack{m \neq a \\ n \neq b}} \frac{\langle a | H_W^{(1)} | m \rangle \langle m | e\alpha_v A^v | n \rangle \langle n | H_W^{(hf)} | b \rangle}{(\varepsilon_a - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} + \sum_{\substack{m \neq a \\ n \neq b}} \frac{\langle a | H_W^{(hf)} | m \rangle \langle m | e\alpha_v A^v | n \rangle \langle n | H_W^{(1)} | b \rangle}{(\varepsilon_a - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} \quad (10) \\
& + \sum_{\substack{m \neq b \\ n \neq b}} \frac{\langle a | e\alpha_v A^v | n \rangle \langle n | H_W^{(1)} | m \rangle \langle m | H_W^{(hf)} | b \rangle}{(\varepsilon_b - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} + \sum_{\substack{m \neq b \\ n \neq b}} \frac{\langle a | e\alpha_v A^v | n \rangle \langle n | H_W^{(hf)} | m \rangle \langle m | H_W^{(1)} | b \rangle}{(\varepsilon_b - \varepsilon_m)(\varepsilon_b - \varepsilon_n)} \\
& - \langle a | H_W^{(hf)} | a \rangle \sum_{\substack{m \neq a \\ n \neq a}} \frac{\langle a | H_W^{(1)} | m \rangle \langle m | e\alpha_v A^v | b \rangle}{(\varepsilon_a - \varepsilon_m)^2} - \sum_{\substack{m \neq b \\ n \neq b}} \frac{\langle a | e\alpha_v A^v | n \rangle \langle n | H_W^{(1)} | b \rangle}{(\varepsilon_b - \varepsilon_n)^2} \langle b | H_W^{(hf)} | b \rangle.
\end{aligned}$$

Here the following notations are used: $|a\rangle = |aI F_F M_F\rangle$, $|b\rangle = |bI F_I M_I\rangle$, 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 $\langle a | PNC | b \rangle^{(a)}$, $\langle a | PNC | b \rangle^{(2)}$ are similar to equation (10). The full description of the corresponding matrix elements and other details of the general method and PC code are presented in refs. [3,4,10, 64-100].

The fundamentals of the RMBPT formalism are presented previously in details in Refs. [41-50] and here we mention only the key points. The RMBPT formalism includes the optimized Dirac-Kohn-Sham (DKS) zeroth approximation and allows to provide an effective taking the relativistic, exchange-correlation, nuclear, radiative effects into account. The relativistic electron wave functions are determined from solution of the relativistic Dirac equation with a general potential.

The latter includes ab initio mean-field potential, electric, polarization potentials of a nucleus. There have been considered all correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, mass operator iterations etc).

A multielectron system is described by the relativistic Dirac Hamiltonian (the atomic units are used) as follows [3,4]:

$$H = \sum_i \{ \alpha c p_i - \beta c^2 - Z / r_i \} + \sum_{i>j} \exp(i | \omega | r_{ij}) (1 - \alpha_i \alpha_j) / r_{ij} \quad (11)$$

where Z is a charge of nucleus, α_i, α_j are the Dirac matrices, ω_{ij} is the transition frequency, c – the velocity of light. The interelectron interaction potential second term in (3)) takes into account the retarding effect and magnetic interaction in the lowest order on parameter of the fine structure constant α^2 (α is the fine structure constant). The mean-field self-consistent potential in the zeroth-order Hamiltonian is as follows:

$$V_{MF} = V^{DKS}(r) = [V_{Coul}^D(r) + V_X(r) + V_C(r|b)] \quad (12)$$

with the standard Coulomb-like potential $V_{Coul}^D(r)$, is the Kohn-Sham exchange potential $V_x(r)$ [39]:

$$V_x[\rho(r),r]=V_x^{KS}(r)\cdot\left\{\frac{3}{2}\ln\frac{[\beta+(\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}}-\frac{1}{2}\right\}, \quad (13a)$$

$$\beta=[3\pi^2\rho(r)]^{1/3}/c \quad (13b)$$

and a correlation functional $V_c(r|b)$, taken in the Lundqvist-Gunnarsson form [4] with ab initio optimization parameter b (for details, see below and Refs. [42,55-60]). The approach includes a generalized procedure (based on a relativistic energy approach) of generating the optimal basis set of relativistic electron wave functions with performance of the gauge invariance principle. To reach the latter we focus on accurate consideration of the QED PT fourth order (a second order of the atomic perturbation theory) Feynman diagrams, whose contribution into imaginary part of radiation width $\text{Im } \delta E$ for the multi-electron ions accounts for multi-body correlation effects. This value is considered to be representative for the correlation effects, whose minimization is a reasonable criterion in the searching for the optimal one-electron basis of the many-body PT. A minimization of the functional $\text{Im } \delta E$ leads to integral-differential Dirac-Kohn-Sham-like density functional equations. The magnetic inter-electron interaction is accounted for in the lowest order on α^2 (α is the fine structure constant) parameter.

The Coulomb-like potential of a nucleus (for the spherically symmetric nuclear density $\rho(r|R)$) is determined as follows:

$$V_{nuc}(r|R)=-\frac{1}{r}\int_0^r dr' r'^2 \rho(r'|R)+\int_r^\infty dr' r' \rho(r'|R) \quad (14)$$

To take into account the radiation (QED) corrections, we used the procedures, described detail in Refs. [41-50,82-87]. A method for calculation of the self-energy part of the Lamb shift is based on an idea by Ivanov-Ivanova et al (e.g. [40]), which generalizes the known hydrogen-like method by Mohr [35] and radiation model potential method by Flambaum-Ginges [36] (look details in Refs. [3,10,61,69,82-87]). According to Ref. [40], the radiative shift and the relativistic part of energy in an atomic system are, in principle, defined by one and the same physical field. One could suppose that there exists some universal function that connects the self-energy correction and the relativistic energy. It is worth to note that the low-energy part of the Lamb shift is determined by the following expression:

$$E_H(\Lambda)=\text{Re}\frac{1}{\pi Z}\int_0^\infty d\xi [E(\xi,0)-E(\xi,\Lambda)], \quad (15a)$$

$$E_H(\xi, \Lambda) = \iint d r_1 d r_2 \frac{1}{r_{12}} \exp\left[(E_0 - i\xi)^2 - \Lambda^2\right]^{1/2} \Psi^+(r_2) \alpha^\mu G(r_1 r_2) \alpha^\mu \Psi(r_1), \quad (15b)$$

(here $\Psi(r)$ is the Dirac function, an energy parameter $E = i\xi$ is imaginary, G is the complex Green's function) and calculated by means of the complex Green function method in version [91]. The important radiation contributions are given by the standard Uehling-Serber term and the Källén-Sabry and Wichmann-Kroll corrections of higher orders (such as $[\alpha(Z\alpha)]^n$ ($n=2, \dots$), $\alpha^2(\alpha Z)$, $\alpha(Z\alpha)^n$ ($n=3$) etc; α is the fine structure constant). In order to take into consideration the effect of the vacuum polarization in the first PT order the generalized Uehling-Serber potential is used and modified to account for the high-order radiative corrections according to the procedure [3]. All calculations are performed with using the numeral codes SuperAtom (Nucleus) (modified versions 93).

3. Results and Conclusions

As the first illustration (the test), we consider ^{133}Cs and present the results (table 1) of calculation of the hyperfine structure (hfs) parameters for Cs. In table 1 the experimental (A^{Exp}) and our ($A^{\text{N-Qed}}$) data for magnetic dipole constant A (MHz) for valent states of ^{133}Cs ($I=7/2$, $g_i=0.7377208$) are presented. The calculation results within standard (A^{RHF}) RHF and RHF with accounting for the second and higher PT corrections, the MCDF approximation and QED formalism are given too (from Refs. [3,22-34,63,69]). The following notations are used: A^{RCC} – calculation by relativistic cluster-coupled (RCC) method; A^{DF} – DF method; A^{RHF} - RHF method and A^{QED} - the QED calculation; $A^{\text{N-Qed}}$ is the result of this work. The key quantitative factor of physically reasonable agreement between theory and experimental data is connected with the correct accounting for the inter electron correlations, nuclear, Breit and QED radiative corrections.

Table 1. The values (MHZ) of the hfs 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]; $A^{\text{N-Qed}}$ – this work

State	A^{MCDF}	A^{RHF}	$A^{\text{RHF}+dA}$	A^{Qed}	$A^{\text{N-Qed}}$	A^{Exp}
$6s_{1/2}$	1736.9	1426.81	2291.00	2294.45	2296.78	2298.16(13)
$6p_{1/2}$	209.6	161.09	292.67	292.102	292.118	291.90(13)

In table 2 the PNC amplitudes (in units of $10^{-11} \text{iea}_B(-Q_W)/N$) are listed and calculated on the basis of the different methods (without the Breit corrections): DF, RHF, MCDF, MBPT and nuclear-RMBPT results (data from refs. [3,22-34,63,69]).

Table 2. PNC amplitudes (in units of $10^{-11}iea_B(-Q_W)/N$), which are calculated by different methods (without the Breit corrections): DF, RHF, MCDF, MBPT and nuclear-QED PT

Atom Trans.	Spin of Nucl.	Nucl. moment μ_N	Radius (fm) of nucleus	DF	RHF	MCDF	MBPT	N-RMBPT
⁸⁵ Rb 5s-6s	5/2	1.3534	4.246	-0.110	-0.138	-0.134	-0.135	-0.132
¹³³ Cs 6s-7s	7/2	2.5826	4.837	-0.741	-0.926 -0.897	-0.904	-0.906 -0.908	-0.903
²²³ Fr 7s-8s	3/2	1.1703	5.640	-13.72	-16.63	-15.72	-15.56 -15.80	-15.54
²¹¹ Fr 7s-8s	9/2	4.0032	5.539	-12.51	-15.16	-14.34	-	-14.17

In table 3 we present the Breit correction (in units of $10^{-11}(-Q_W)/N$) to the PNC amplitude, which are calculated by the different methods (without the Breit corrections): DF, RHF, MCDF, and nuclear-RMBPT (data from Refs. [3,22-34,63,69]). Let us note that the radiative corrections to the PNC amplitude, provided by the vacuum-polarization (VP) effect and the self-energy (SE) part are as follows: $E_{PNC} - {}^{133}\text{Cs}$ - VP=0.38%, SE=-0.74%; ${}^{223}\text{Fr}$ - VP=1.025%, SE=-1.35%.

Table 3. The Breit correction (in units of $10^{-11}(-Q_W)/N$) to the PNC amplitude, which are calculated by the different methods (without the Breit corrections): DF, RHF, MCDF, and nuclear-RMBPT results (other data from refs. [25,29,33])

Atom: Transition	DF	RHF	MCDF	N-QED PT
¹³³ Cs 6s-7s	0.0022	0.0018	0.0045	0.0049
²²³ Fr 7s-8s	0.0640	0.0650	0.1430	0.1703

In table 4 we list the nuclear spin dependent corrections to PNC (${}^{133}\text{Cs}$: 6s-7s) amplitude, calculated by different theoretical methods (in units of the $k_{a,2,hf}$ coefficient): MBPT, DF-PT, the shell model, N-RMBPT (from Refs. [3,22-34,63,69]).

Table 4. The nuclear spin-dependent corrections to the PNC ^{133}Cs : 6s-7s amplitude E_{PNC} , calculated by different methods (in units of $k_{a,2,\text{hf}}$ coeff.): MBPT, DF-PT, shell model, N-RMBPT (see text)

Correction	MBPT	Shell model	DF	N-RMBPT
K (sum)	0.1169	0.1118	0.112	0.1159
k_2 - the Z-boson exchange interaction from nucleon axial-vector currents ($A_n V_e$)	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

In table 5 we present the estimated values of the weak charge Q_w for different heavy atoms, predicted in different approaches and determined in the Standard model (SM) (from Rrefs. [1-7,22-34,63,69]). The analysis of results shows that in principle a majority of theoretical approaches provide physically reasonable agreement with the Standard model data, but the important question is how much exact this agreement is. Some received data on estimating these constants directly indicate the necessity of new adequate précised experiments. The rare-earth elements (and corresponding multicharged ions), in particular, ytterbium, are especially interesting as they have very complicated spectra of energy levels with very unusual behavior in relatively weak electric and laser fields. In our opinion, particular attention should be paid to the ^{173}Yb ytterbium atom, where the theoretical PNC values of the EPNC amplitude differ from similar values of all considered heavy alkaline atoms by almost two orders of magnitude, which makes this atom particularly important in terms of studying the weak electron-nuclear interaction, the PNC effect, and of course, the Standard model check. Excessive complexity of the ^{173}Yb calculation, where the correlation effects corrections (including quick “blurring” of the initial state over an infinite set of additional configurations and other effects) is very large, making it difficult to obtain data on the fundamental parameters of Yb. Using the experimental value $\Delta E_1^{\text{PNC}}/\beta$ [11]: $(8.7 \pm 1.4) \cdot 10^{-10} \text{ea}_B$ ($\Delta E_1^{\text{PNC}}/\beta = 39 \text{ mV/cm}$) and the calculated atomic constant value of $99.707 \cdot 10^{-10} \text{ea}_B$ (for ^{173}Yb ; $Z = 70$, $N = 103$)

Table 5. The estimated values of the weak charge Q_W and final PNC amplitudes (in units $10^{-11}iea_B(-Q_W)/N$) for different heavy atoms, predicted in different approaches

Contribution	E_{PNC} Q_W	N- RMBPT	MCDF	MBPT- DF	MCDF- QED	RHF+Breit+ Correlation	RCC
$^{85}\text{Rb } 5s-6s$	E_{PNC}	-0.1318	-0.135	-	-	-0.134	-
$^{133}\text{Cs } 6s-7s$	E_{PNC}	-0.8985	-0.935	-0.897	-0.8981	-0.898	-0.9054
			-0.905	-0.904	-0.9055	-0.910	-0.899
						-0.902	
$^{133}\text{Cs } 6s-7s$ $Q_W^{SM} = -73.19(13)$	Q_W	-72.62	-69.78	-72.69	-72.65	-72.66	-72.06
			-71.09	-72.18	-72.06	-71.70	-72.58
						-72.42	
$^{137}\text{Ba}^+$ $6s-5d_{3/2}$	E_{PNC}	-2.385	-	-2.35	-	-2.34	-2.46
^{173}Yb $6s^{21}S_0-$ $5d6s^3D_1$ $Q_W^{SM} = -95.44(8)$	E_{PNC} Q_W	-97.07 -92.31	-	-	-	-	-
			-	-	-	-	-
^{205}Tl $6p_{1/2}-6p_{3/2}$	E_{PNC}	26.5114	-26.75	-26.5	-	-	-
^{205}Tl $6p_{1/2}-6p_{3/2}$ $Q_W^{SM} = -116.81(4)$	Q_W	-116.55	-112.4	-116.2 -116:7	-	-	-

it is not difficult to determine the value of a weak charge $Q_W = -92.31$, which is different from Q_W (the Standard model) = -95.44. This circumstance imposes unambiguous restrictions on the fundamental values of S, T. It is interesting to note that the estimate of difference $[Q_W \text{ (theoretical)} - Q_W \text{ (CM)}] \sim 6$ indicated in [11] in our opinion, is a little overestimated due to the neglect of the contribution of QED, neutron skin effects etc. Perhaps the increase in the PNC effect at ^{173}Yb can be explained qualitatively and quantitatively in terms of a quantum chaos theory and strong inter-electron correlations (e.g.[3,100]). In any case, it is worth noting the "sensitivity" of PNC experiments to New Physics at energies, which even today are difficult to reach on modern colliders, including the restrictions on the mass of the Z boson and the mixing angle in models beyond the Standard model.

The analysis shows that the perspectives of the PNC experiments with Stark pumping of the individual states in the rare-earth atoms (and probably more effective multicharged ions of these elements) and simultaneously polarized laser field dressing (with a cold-atom fountain or interferometer) may provide comfortable conditions for precise observation of weak effects.

II. Task options for self-sufficient work

Task Option 1.

- 1). Give the key definitions of a theoretical approach to definition of Hyperfine and electroweak interaction parameters in heavy finite Fermi systems and the characteristics of effect of non-conservation of parity: i) mathematical and physical essence of electroweak interaction parameters in heavy finite Fermi systems, ii) mathematical and physical essence of hyperfine interaction parameters in heavy finite Fermi systems iii) mathematical and physical essence of effect of non-conservation of parity, iv) QED-nuclear perturbation theory for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems, v) analysis of the role of nuclear, exchange-correlation effects, relativistic and radiative effects for relativistic atoms and multicharged ions. Explain all definitions in **QED-nuclear perturbation theory** for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems on the example of the caesium, rubidium and other alkali atoms;
- 2). To apply the preliminarily describing the corresponding spectrum of a free system, i.e. without an external electric field, say, **lanthanide atom of Yb**. To perform its practical realization (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark" for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

Task Option 2.

- 1). Give the key definitions of a theoretical approach to definition of Hyperfine and electroweak interaction parameters in heavy finite Fermi systems and the characteristics of effect of non-conservation of parity: i) mathematical and physical essence of electroweak interaction parameters in heavy finite Fermi systems, ii) mathematical and physical essence of hyperfine interaction parameters in heavy finite Fermi systems iii) mathematical and physical essence of effect of non-conservation of parity, iv) QED-nuclear perturbation theory for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems, v) analysis of the role of nuclear, exchange-correlation effects, relativistic and radiative effects for relativistic atoms and multicharged ions. Explain all definitions in **QED-nuclear perturbation theory** for

calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems on the example of the caesium, rubidium and other alkali atoms;

2). To apply the preliminarily describing the corresponding spectrum of a free system, i.e. without an external electric field, say, **lanthanide atom of Tm**. To perform its practical realization (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark" for quantum system from the first task of the option (all necessary numerical parameters should be self-taken)).

Task Option 3.

1). Give the key definitions of a theoretical approach to definition of Hyperfine and electroweak interaction parameters in heavy finite Fermi systems and the characteristics of effect of non-conservation of parity: i) mathematical and physical essence of electroweak interaction parameters in heavy finite Fermi systems, ii) mathematical and physical essence of hyperfine interaction parameters in heavy finite Fermi systems iii) mathematical and physical essence of effect of non-conservation of parity, iv) QED-nuclear perturbation theory for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems, v) analysis of the role of nuclear, exchange-correlation effects, relativistic and radiative effects for relativistic atoms and multicharged ions. Explain all definitions in **QED-nuclear perturbation theory** for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems on the example of the caesium, rubidium and other alkali atoms;

2). To apply the preliminarily describing the corresponding spectrum of a free system, i.e. without an external electric field, say, **lanthanide atom of La**. To perform its practical realization (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark" for quantum system from the first task of the option (all necessary numerical parameters should be self-taken)).

Task Option 4.

1). Give the key definitions of a theoretical approach to definition of Hyperfine and electroweak interaction parameters in heavy finite Fermi systems and the characteristics of effect of non-conservation of parity: i) mathematical and

physical essence of electroweak interaction parameters in heavy finite Fermi systems, ii) mathematical and physical essence of hyperfine interaction parameters in heavy finite Fermi systems iii) mathematical and physical essence of effect of non-conservation of parity, iv) QED-nuclear perturbation theory for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems, v) analysis of the role of nuclear, exchange-correlation effects, relativistic and radiative effects for relativistic atoms and multicharged ions. Explain all definitions in **QED-nuclear perturbation theory** for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems on the example of the caesium, rubidium and other alkali atoms;

2). To apply the preliminarily describing the corresponding spectrum of a free system, i.e. without an external electric field, say, **lanthanide atom of Gd**. To perform its practical realization (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark" for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

Task Option 5.

1). Give the key definitions of a theoretical approach to definition of Hyperfine and electroweak interaction parameters in heavy finite Fermi systems and the characteristics of effect of non-conservation of parity: i) mathematical and physical essence of electroweak interaction parameters in heavy finite Fermi systems, ii) mathematical and physical essence of hyperfine interaction parameters in heavy finite Fermi systems iii) mathematical and physical essence of effect of non-conservation of parity, iv) QED-nuclear perturbation theory for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems, v) analysis of the role of nuclear, exchange-correlation effects, relativistic and radiative effects for relativistic atoms and multicharged ions. Explain all definitions in **QED-nuclear perturbation theory** for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems on the example of the caesium, rubidium and other alkali atoms;

2). To apply the preliminarily describing the corresponding spectrum of a free system, i.e. without an external electric field, say, **lanthanide atom of Eu**. To perform its practical realization (using Fortran Power Station, Version 4.0; PC

Code: “Superatom-Stark” for quantum system from the first task of the option (all necessary numerical parameters should be self-taken).

Task Option 6.

1). Give the key definitions of a theoretical approach to definition of Hyperfine and electroweak interaction parameters in heavy finite Fermi systems and the characteristics of effect of non-conservation of parity: i) mathematical and physical essence of electroweak interaction parameters in heavy finite Fermi systems, ii) mathematical and physical essence of hyperfine interaction parameters in heavy finite Fermi systems iii) mathematical and physical essence of effect of non-conservation of parity, iv) QED-nuclear perturbation theory for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems, v) analysis of the role of nuclear, exchange-correlation effects, relativistic and radiative effects for relativistic atoms and multicharged ions. Explain all definitions in **QED-nuclear perturbation theory** for calculation of energy and radiation transition amplitudes parameters in heavy finite Fermi systems on the example of the caesium, rubidium and other alkali atoms;

2). To apply the preliminarily describing the corresponding spectrum of a free system, i.e. without an external electric field, say, **lanthanide atom of Sm**. To perform its practical realization (using Fortran Power Station, Version 4.0; PC Code: “Superatom-Stark” for quantum system from the first task of the option (all necessary numerical parameters should be self-taken)).

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