МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Computational Methods of dynamics of classical and quantum systems. Part 7". (Training of PhD students of the specialty: 113 – "Applied mathematics" and others)

«Затверджено»
на засіданні групи забезпечення спеціальності
Протокол №1 від 28/08/2021 Голова групи _____Хецеліус О.Ю.

«Затверджено»
на засіданні кафедри вищої та прикладної математики
Протокол №1 від 28/08/2021 Зав. кафедри _____Лушков О.В.

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THE MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE
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Odessa 2021

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PREFACE

Discipline "Computational methods of dynamics of classical and quantum systems" is a compulsory discipline in the cycle of professional training of postgraduate students (3 level of education) in specialty 113 - Applied mathematics.

It is aimed at assimilating (assuring) a number of planned competences, including developing fundamentally new and to improve the existing modern computational methods and algorithms of quantum mechanics, geometry and electrodynamics for the analysis, modeling and prediction of the properties of classical and quantum systems with pronounced resonance behavior, the ability to analyze data of computer experiments on the study of the characteristics of quantum systems that can be large and require the use of powerful computing resources, the use of modern existing and new advanced computational methods in order to achieve scientific results that create potentially new knowledge in computational mathematics.

The place of discipline in the structural-logical scheme of its teaching: the knowledge gained during the study of this discipline is used in the writing of dissertations, the topics of which are related to the development of new computing methods and algorithms dynamics of complex chaotic systems with possible generalizations on various classes of mathematical, physical and chemical, cybernetic, socio-economic, ecological systems.

The basic concepts of discipline are the fundamental tools of a specialist in the field of applied mathematics.

The purpose of studying the discipline is assimilation (assurance) of a number of competencies, in particular, the achievement of the relevant knowledge, mastering the modern apparatus of quantum geometry and resonance theory, the ability to develop new and improve existing mathematical methods for the analysis, modeling and prediction of spectral properties of quantum systems on the basis of the apparatus of quantum mechanics, geometry and electrodynamics, the search for new resonance phenomena in the dynamics of quantum systems, etc.

After mastering this discipline, the postgraduate student must be able to use modern or personally developed new computing methods, in particular, to analyze, simulate, predict, and program the resonant dynamics of classical and quantum systems with the formulation of appropriate computer experiments

These methodical instructions are for the first-year PhD students and tests performance in the discipline Computational methods of dynamics of classical and quantum systems". The main topic: Numerical foundations of relativistic (QED) multiparticle perturbation theory in problems of quantum geometry, mechanics, dynamics ...

Topic: Numerical foundations of relativistic (QED) multiparticle perturbation theory in problems of quantum geometry, mechanics, dynamics ...

Topic: Чисельні основи релятивістської (КЕД) багаточастинкової теорії збурень в задачах квантової геометрії, механіки, динаміки.. (ЗБЛ4)

1. Introduction

Different topics of the modern physics of electroweak interactions are now a subject of intensive theoretical and experimental interest. From the other side, the parity violation (non-conservation) experiments in atomic physics provide an important possibility to deduce information on the Standard Model independently of high-energy physics experiments [1-8]. The recent LEP experiments are fulfilled [1,2], that yield extremely accurate values for Z-boson properties. 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. 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 fundamental purposes of the high-precision atomic PNC studies are to search for new physics beyond the SM of the electroweak interaction by precise evaluation of the weak charge Q_W and to probe parity violation in the nucleus by evaluation of the nuclear anapole moment. The detailed review of these topics can be found in refs. [1-10], 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.

The most popular multiconfiguration Dirac-Fock (MCDF) method for calculating parity and time reversal symmetry violations in many-electron atoms has some serious disadvantages [3,17,26]. This fact has stimulated a development of different versions of the many-body perturbation theory (PT), namely, the PT with relativistic Hartree-Fock (RHF) and DF zeroth approximations, QED-PT and nuclear-QED PT [11-44].

In present paper the new theoretical approach, namely, nuclear-QED PT is used for detection of the hyperfine structure and electroweak interaction parameters, scalar-pseudoscalar interaction constant and parity non-conservation (PNC) effect in atomic system. In fact the N-QED PT is based on the combining ab initio QED PT formalism and nuclear relativistic middle-field (RMF) model and allows to fulfil studying the spectra for atomic systems with an account of the relativistic, correlation, nuclear, radiative effects [10,38-44]. 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 [10]. The results of studying the different atomic systems are presented.

2. Nuclear-QED PT approach to electroweak interactions in heavy finite Fermi-systems and parity-non-conservation transition amplitude determination

The wave electron functions zeroth basis is found from the Dirac equation solution with potential, which includes the core ab initio potential, electric, polarization 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. Though we have no guaranty that these wave-functions yield a close approximation to nature, the success of the RMF approach supports our choice [35]. These wave functions do not suffer from known deficiencies of other approaches, e.g., the wrong asymptotics of wave functions obtained in a harmonic oscillator potential. The RMF model has been designed 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. [35]), its ansatz is a Lagrangian or Hamiltonian that incorporates the effective, in-medium nucleon-nucleon interaction. Recently the self-consistent models have undergone a reinterpretation, which explains their quantitative success in view of the facts that nucleons are composite objects and that the mesons employed in RMF have only a loose correspondence to the physical meson spectrum. They are seen as covariant Kohn-Sham schemes and

as approximations to the true functional of the nuclear ground state. As a Kohn-Sham scheme, the RMF model can incorporate certain ground-state correlations and yields a ground-state description beyond the literal mean-field picture. RMF models are effective field theories for nuclei below an energy scale of 1GeV, separating the long- and intermediate-range nuclear physics from short-distance physics, involving, i.e., short-range correlations, nucleon form factors, vacuum polarization etc, which is absorbed into the various terms and coupling constants.

In our approach we have used so called NL3-NLC and generalized Ivanov et al approach (see details in refs. [4,12]), 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 the total potential *V(r)*. 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 total potential includes the electric potentials of a nucleus with using the RNF charge distribution, exchange-correlation and radiative potentials. The radiative QED (the self-energy part of the Lamb shift and the vacuum polarization contribution in the lower order plus corrections of the high QED orders) are accounted for within the QED formalism [4]. The continuum pressure effects and contribution of the autionization states are taken onto account by means the Dirac-Sturm approach. The full description of the corresponding models and other details of the general method are presented in refs.[4,10,39-44].

Below we are limited by presenting the key formulae for determination of 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 [5]:

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

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

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, m_W is the mass of the W boson, $\rho(r)$ 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 as follows:

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

The latter can be rewritten with accounting for the radiative corrections as [5,18]:

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

$$\sin^2\theta_W = 0.2323 + 0.00365S - 0.00261T) \qquad (3)$$

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 ((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_nV_e), and the combined action of the hyperfine interaction and spin-independent Z-boson exchange from nucleon vector (V_nA_e) currents [7,9,34]. The anapole moment contribution strongly dominates.

The above-mentioned interactions can be represented by the Hamiltonian

$$H_W^i = \frac{G_F}{\sqrt{2}} k_i(\alpha\cdot I)\rho(r) \qquad (4)$$

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 [10]:

$$< i \mid H_W^1 \mid j >= i \frac{G_F}{2\sqrt{2}} Q_W \delta_{k_i - k_j} \delta_{m_i m_j} \int_0^\infty dr[F_i(r)G_j(r) - G_i(r)F_j(r)]\rho(r) \qquad (5)$$

The reduced matrix element is as follows:

$$< i \parallel H_W^1 \parallel j >= i \frac{G_F}{2\sqrt{2}} Q_W \int_0^\infty dr[F_i(r)G_j(r) - G_i(r)F_j(r)]\rho(r) \qquad (6)$$

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

$$< a \mid PNC \mid b >= -\sum_n [\frac{< b \mid e\alpha_\nu A^\nu \mid n >< n \mid H_W^{(1)} \mid a >}{\varepsilon_a - \varepsilon_n} + \frac{< b \mid H_W^{(1)} \mid n >< n \mid e\alpha_\nu A^\nu \mid a >}{\varepsilon_b - \varepsilon_n} \qquad (7)$$

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).

The corresponding spin-dependent PNC contribution is as follows:

$$< a \mid PNC \mid b >^{sd} = k_a < a \mid PNC \mid b >^{(a)} + k_2 < a \mid PNC \mid b >^{(2)} + k_{hf} < a \mid PNC \mid b >^{(hf)} \quad (8)$$

It should be noted the expressions for the matrix elements $< a \mid PNC \mid b >^{(a)}$ and others in Eq. (8) are similar to equation (12), however have much more complicated form.

3. Results and future prospects

In table 1 we listed the calculated and experimental values of the hyperfine structure (hfs) energy and magnetic moments (in nuclear magnetons) in the $^{207}Tl^{80+}$, which are determined within the nuclear–QED theory and other different theoretical models [12-14]. The key quantitative factor of agreement between our N-QED theory and experimental data is connected with the correct accounting for the inter electron correlations, nuclear, Breit and QED radiative corrections (including magnetic moment distribution in a nucleus and nuclear corrections).

Table 1. The hfs energy and magnetic moment (in nuclear magnetons) in $^{207}Tl^{80+}$ [12-14]

Magn. moment [μ_N]	HS NLC Tomaselli N-QED
Theory Exp. [14]	1.8769 1.8758 1.6472 1.8764 1.8765(5)
HFS[eV]	HS NLC Tomaselli N-QED
ΔE^1_{HFS} ΔE_{QED}	3,721 3,729 3,2592 3,5209 -0,0201 -0,0178 -0,0207
Total	3,701 3,708 3,2592 3,5002

In table 2 there are listed the PNC amplitudes (in units of $10^{-11}iea_B(-Q_W)/N$) for a number of radiative transitions in spectra of the Cs, Tl, Yb isotopes, which are calculated by the different methods (without the Breit corrections): DF, RHF, MCDF, many-body perturbation theory (MBPT) and our nuclear-QED PT results (other data from refs. [25-34]).

Table 2. The PNC amplitudes (in units of $10^{-11}iea_B(-Q_W)/N$) and estimated values of the weak
charge Q_W for different heavy atoms, predicted in different approaches (see text)

Isotope, transition	**E_{PNC} Q_W**	N-QED	MCDF	MBPT-DF	MCDF-QED	TDRHF-C	RCC
^{133}Cs 6s-7s	E_{PNC}	-0.8985	-0.935 -0.905	-0.897 -0.904	-0.8981 -0.9055	-0.898 -0.910 -0.902	- 0.9054 -0.899
^{133}Cs 6s-7s $Q_W^{SM} = -73.19$	**Q_W**	**-72.62**	**-69.78** **-71.09**	**-72.69** **-72.18**	**-72.65** **-72.06**	**-72.66** **-71.70** **-72.42**	**-72.06** **-72.58**
^{173}Yb **$6s^2{}^1S_0$-$5d6s^3D_1$** $Q_W^{SM} = -95.44$	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 $6p_{1/2}$-$6p_{3/2}$ $Q_W^{SM} = -116.81$	**Q_W**	**-116.15**	**-112.4**	**-116.2**	-	-	-

Let us underline that the values of the weak charge are firstly predicted by us for ^{173}Yb atoms. The analysis of results shows that in principle a majority of theoretical approaches provides physically reasonable agreement with the Standard model data, but the important question is how much exact this agreement. In our opinion, however, the précised estimates indicate on the tiny deviation from the Standard model. In any case analysis of the data allow to conclude that the SM violation has a place, however it can be hardly stated on significant violation. Nevertheless, one could turn to attention on the "sensibility" of the PNC experiments to New Physics for energies, which are hardly reached at the modern colliders. This fact is clearly illustrated by the figure 1, where the darkled region is eliminated from the measurements in the PNC and colliders experiments.

Therefore, in this paper we presented new more accurate data on some fundamental hyperfine and electroweak constants in the Cs, Tl and Yb isotopes using a new approach to determination of the electroweak and hyperfine interactions parameters and parity non-conservation effect in heavy atomic and

nuclear systems, based on the combined QED perturbation theory formalism and relativistic nuclear mean-field theory. Some listed data on the indicated constants directly stimulate carrying out new sufficiently précised experiments in order to provide the low-energy test of the Standard Model. The rare-earth elements have to be especially interesting as they have very complicated spectra of autoionization resonances (with very unusual from physical point of view their behavior in a weak electric and laser fields; the known effect of resonances giant

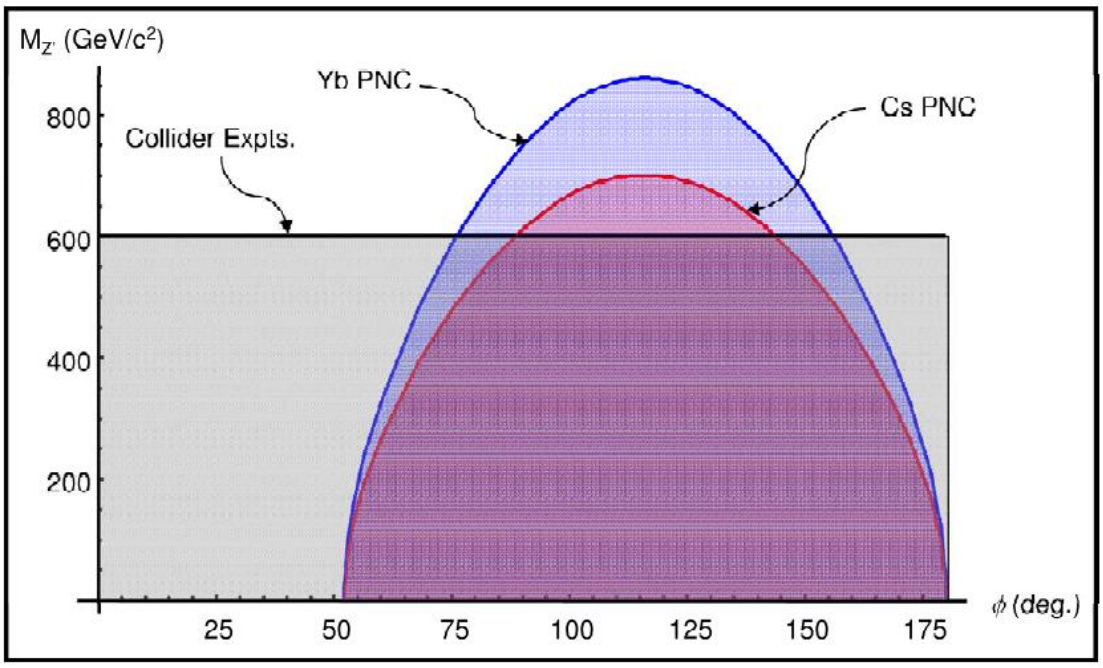

Figure 1. The limitations on the Z' boson mass and missing angle in the models beyond the Standard Model (see comment in the text).

broadening [4]). The elementary comments show that the prospects of the PNC experiments with Stark pumping (or a polarization plane rotation) of the individual states (in the considered isotopes,
including the rare-earth elements; probably more effective possibility is given by studying multicharged ions of these elements) and simultaneously polarized laser field dressing (with a cold-atom fountain or interferometer) could provide comfortable conditions for précised experimental observation of the weak effects.

4. Task options

Task Option 1.

1). Give the key definitions in relativistic (QED) multiparticle perturbation theory in problems of quantum geometry: i) mathematical and physical essense of perturbation theory corrections, ii) Operator of the perturbation iii) block of the correlatio corrections iii) block of radiative QED corrections, iv) block of nthe nuclear corrections v) hyperfine and electroweak interactions vi) parity non-conservation amplitudes in heavy finite fermi-systems vii). the technical details of the computation code.

2) Explain all definitions of hyperfine and electroweak interactions parameters and parity non-conservation amplitudes in heavy atoms (**caesium**).

3). To carry out the numerical algorythm for computing key characteristics using the Runge-Cutta methods. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” for the example 3 (all necessary numerical parameters should be self-taken).

Task Option 2.

1). Give the key definitions in relativistic (QED) multiparticle perturbation theory in problems of quantum geometry: i) mathematical and physical essense of perturbation theory corrections, ii) Operator of the perturbation iii) block of the correlatio corrections iii) block of radiative QED corrections, iv) block of nthe nuclear corrections v) hyperfine and electroweak interactions vi) parity non-conservation amplitudes in heavy finite fermi-systems vii). the technical details of the computation code.

2) Explain all definitions of hyperfine and electroweak interactions parameters and parity non-conservation amplitudes in heavy atoms (**radium**).

3). To carry out the numerical algorythm for computing key characteristics using the Runge-Cutta methods. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” for the example 3 (all necessary numerical parameters should be self-taken).

Task Option 3.

1). Give the key definitions in relativistic (QED) multiparticle perturbation theory in problems of quantum geometry: i) mathematical and physical essense of perturbation theory corrections, ii) Operator of the perturbation iii) block of the correlatio corrections iii) block of radiative QED corrections, iv) block of nthe nuclear corrections v) hyperfine and electroweak interactions vi) parity non-conservation amplitudes in heavy finite fermi-systems vii). the technical details of the computation code.
2) Explain all definitions of hyperfine and electroweak interactions parameters and parity non-conservation amplitudes in heavy atoms (**ytterbium**).
3). To carry out the numerical algorythm for computing key characteristics using the Runge-Cutta methods. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” for the example 3 (all necessary numerical parameters should be self-taken).

Task Option 4.

1). Give the key definitions in relativistic (QED) multiparticle perturbation theory in problems of quantum geometry: i) mathematical and physical essense of perturbation theory corrections, ii) Operator of the perturbation iii) block of the correlatio corrections iii) block of radiative QED corrections, iv) block of nthe nuclear corrections v) hyperfine and electroweak interactions vi) parity non-conservation amplitudes in heavy finite fermi-systems vii). the technical details of the computation code.
2) Explain all definitions of hyperfine and electroweak interactions parameters and parity non-conservation amplitudes in heavy atoms (**uranium**).
3). To carry out the numerical algorythm for computing key characteristics using the Runge-Cutta methods. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” for the example 3 (all necessary numerical parameters should be self-taken).

Task Option 5.

1). Give the key definitions in relativistic (QED) multiparticle perturbation theory in problems of quantum geometry: i) mathematical and physical essense of perturbation theory corrections, ii) Operator of the perturbation iii) block of the correlatio corrections iii) block of radiative QED corrections, iv) block of nthe nuclear corrections v) hyperfine and electroweak interactions vi) parity non-conservation amplitudes in heavy finite fermi-systems vii). the technical details of the computation code.
2) Explain all definitions of hyperfine and electroweak interactions parameters and parity non-conservation amplitudes in heavy atoms (**francium**).
3). To carry out the numerical algorythm for computing key characteristics using the Runge-Cutta methods. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” for the example 3 (all necessary numerical parameters should be self-taken).

Task Option 6.

1). Give the key definitions in relativistic (QED) multiparticle perturbation theory in problems of quantum geometry: i) mathematical and physical essense of perturbation theory corrections, ii) Operator of the perturbation iii) block of the correlatio corrections iii) block of radiative QED corrections, iv) block of nthe nuclear corrections v) hyperfine and electroweak interactions vi) parity non-conservation amplitudes in heavy finite fermi-systems vii). the technical details of the computation code.
2) Explain all definitions of hyperfine and electroweak interactions parameters and parity non-conservation amplitudes in heavy atoms (**gadolinium**).
3). To carry out the numerical algorythm for computing key characteristics using the Runge-Cutta methods. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” for the example 3 (all necessary numerical parameters should be self-taken).

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