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RELATIVISTIC THEORY OF SPECTRA OF PIONIC ATOMS WITH ACCOUNT OF THE RADIATIVE AND NUCLEAR CORRECTIONS

A new theoretical approach to the description of spectral parameters pionic atoms in the excited states with precise accounting relativistic, radiation, nuclear, electron screening effects on the basis of the relativistic Klein-Gordon-Fock equation and QED perturbation theory formalism is developed. A consistent relativistic theory of hyperfine structure of spectra for the pionic atoms is presented. Numerical data on the electromagnetic contributions to the transition energies in spectra of different pionic atoms are listed.

1. Introduction

Our work is devoted to the development of a new theoretical approach to the description of spectral parameters pionic atoms in the excited states with precise accounting relativistic, radiation, nuclear, electron screening effects on the basis of Klein-Gordon-Fock equation and a development of a consistent relativistic theory of hyperfine structure of spectra. There are calculated energies of X-ray np-1s (n=2-4) transitions in the pionic hydrogen spectrum, 5g-4f, 5f-4d, transitions, hyperfine structure levels energies and probabilities in pionic nitrogen, 6h-5g, 6g-5f transitions for pionic Ne, transitions energies in the spectra of middle and heavy pionic atoms (such as ^{133}Ss , ^{175}Lu , ^{181}Ta , ^{205}Tl , ^{202}Pb , ^{238}U) with precise accounting radiation (vacuum polarization), nuclear, electron screening effects. As introduction let us remind that at present time studying the exotic hadronic atomic systems such as pionic atoms is of a great interest for further development of atomic and nuclear theories as well as new tools for sensing the nuclear structure and fundamental pion-nucleus strong interactions. In the last few years transition energies in pionic atoms [1] have been measured with an unprecedented precision. Besides, light pionic atoms can additionally be used as a new low-energy X-ray standards [1]. More over, their spectra studying allows to determine the pion mass using the high-

est accuracy in comparison with other methods. TO nowadays, new advanced experiments are been preparing in order to make sensing the electromagnetic and strong interaction effects in different pionic atoms.

The most popular theoretical models are naturally (pion is the Boson with spin 0, mass $m_{\pi^-} = 139.57018 \text{ MeV}$, $r_{p^-} = 0.672 \pm 0.08 \text{ fm}$) based on the using the Klein-Gordon-Fock equation, but there are many important problems connected with accurate accounting for as pion-nuclear strong interaction effects as QED radiative corrections (firstly, the vacuum polarization effect etc.). This topic has been a subject of intensive theoretical and experimental interest (see [1-14]). The perturbation theory expansion on the physical; parameter αZ is usually used to take into account the radiative QED corrections, first of all, effect of the polarization of electron-positron vacuum etc. This approximation is sufficiently correct and comprehensive in a case of the light pionic atoms, however it becomes incorrect in a case of the heavy atoms with large charge of a nucleus Z . So, there is a high necessity to develop non-perturbative methods in order to account the QED effects. Besides, let us underline that more correct accounting of the finite nuclear size and electron-screening effects for heavy pionic atoms is also very serious and actual problem. At last, a development of the comprehensive theory of

hyperfine structure is of a great interest and importance in a modern theory of the pionic atom spectra.

2. New relativistic theory of pionic atoms with accounting the radiative, nuclear, electron-screening and hyperfine structure effects

As usually, the relativistic dynamic of a spinless boson particle should be described on the basis of the Klein-Gordon-Fock (KGF) equation. The electromagnetic interaction between a negatively charged pion and the atomic nucleus can be taken into account introducing the nuclear potential A_v in the KG equation via the minimal coupling $p_v \rightarrow p_v - qA_v$. The wave functions of the zeroth approximation for pionic atoms are determined from the KGF equation [1]:

$$m^2 c^2 \Psi(x) = \left\{ \frac{1}{c^2} [i\hbar \partial_t + eV_0(r)]^2 + \hbar^2 \nabla^2 \right\} \Psi(x) \quad (1)$$

where \hbar is the Planck constant, c the velocity of the light and the scalar wavefunction $\Psi_0(x)$ depends on the space-time coordinate $x = (ct, r)$. Here it is considered a case of a central Coulomb potential $(V_0(r), 0)$. Here we consider the stationary solution of (1) and represent the wave function as follows:

$$\Psi(x) = \exp(-iEt/\hbar) \varphi(x). \quad (2)$$

Resulting master equation looks as:

$$\left\{ \frac{1}{c^2} [E + eV_0(r)]^2 + \hbar^2 \nabla^2 - m^2 c^2 \right\} \varphi(x) = 0 \quad (3)$$

where E is the total energy of the system (sum of the mass energy mc^2 and binding energy e_0). In principle, the central potential V_0 should include the central Coulomb potential, the radiative (in particular, vacuum-polarization) potential as well as the electron-screening potential in the atomic-optical (electromagnetic) sector. Surely, the full solution of the pionic atom energy especially for the low-excited state requires an inclusion the pion-nuclear strong interaction potential. However, if a pion is on the high orbit of the atom, the strong interaction effects can not be accounted because of the negligible value.

The solution of the Eq. (3) can be resulted in system of the differential equations as follows:

$$\frac{d}{dr} p = q, \quad (4)$$

$$\frac{d}{dr} q = \left[\mu c^2 + \frac{l(l+1)}{r^2} - \alpha^2 (V_c - E)^2 \right] p \quad (5)$$

where p is the radial part of the pion wave function.

The important nuclear effect is the finite size one (the Breit-Rosenthal-Crawford-Schawlow effect). We will use the widespread Gaussian model for nuclear charge distribution. This is the smooth function, and as result it has a advantage in comparison with usually used model of a uniformly charged sphere [2-5]. It is obvious that it simplifies the calculation procedure and permits to perform a flexible simulation of the real distribution of the charge in a nucleus. Another variant for the nuclear charge distribution function is given by the known Fermi model. Within this model the charge distribution in the nucleus $\rho(r)$ is defined as (c.f.[15]):

$$\rho(r) = \rho_0 / \{1 + \exp[(r - c)/a]\} \quad (6)$$

where the parameter $a = 0.523$ fm, the parameter c is chosen by such a way that it is true the following condition for average-squared radius:

$$\langle r^2 \rangle^{1/2} = (0.836 \times A^{1/3} + 0.5700) \text{ fm.}$$

The Gauss model is determined as follows:

$$\rho(r|R) = (4\gamma^{3/2}/\sqrt{\pi}) \exp(-\gamma r^2), \quad (7)$$

where $\gamma = 4\pi/R^2$, R is an effective radius of a nucleus.

Further let us present the formulas for the finite size nuclear potential (its derivatives on the nuclear radius). If the point-like nucleus has the central potential $W(R)$, then a transition to the finite size nuclear potential is realized by exchanging $W(r)$ by the potential [16]:

$$W(r|R) = W(r) \int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r'^2 W(r') \rho(r'|R). \quad (8)$$

We assume it as some zeroth approximation. Further the derivatives of various characteristics on R are calculated. They describe the interaction of the nucleus with outer electron; this permits recalculation of results, when R varies within reasonable limits. The Coulomb potential for the spherically symmetric density $\rho(r|R)$ is:

$$V_{FS}(r|R) = -\left(\frac{1}{r}\right) \int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r' \rho(r'|R) \quad (9)$$

It is determined by the following system of differential equations (for the Fermi model) [16]:

$$V'_{FS}(r, R) = \left(\frac{1}{r^2}\right) \int_0^r dr' r'^2 \rho(r', R) \equiv \left(\frac{1}{r^2}\right) y(r, R)$$

$$y'(r, R) = r^2 \rho(r, R) \quad (10)$$

$$\rho'(r) = (\rho_0/a) \exp[(r-c)/a] \cdot \{1 + \exp[(r-c)/a]\}^2$$

with the corresponding boundary conditions.

The next important topic is connected with a correct accounting the radiation QED corrections and, first of all, the vacuum polarization correction. We firstly introduce into the theory the Flambaum-Ginges radiative potential. It includes the standard Ueling-Serber potential and electric and magnetic form-factors plus potentials for accounting of the high order QED corrections such as [15]

$$\Phi_{rad}(r) = \Phi_U(r) + \Phi_g(r) + \Phi_f(r) + \Phi_l(r) + \frac{2}{3} \Phi_U^{high-order}(r) \quad (11)$$

where

$$\Phi_U^{high-order}(r) = -\frac{2\alpha}{3\pi} \Phi(r) \frac{0.092Z^2\alpha^2}{1 + (1.62r/r_C)^4} \quad (12)$$

$$\Phi_l(r) = -\frac{B(Z)}{e} Z^4 \alpha^5 mc^2 e^{-Zr/a_B} \quad (13)$$

Here e —a proton charge and universal function $B(Z)$ is defined by expression: $B(Z) = 0.074 + 0.35Za$. The corresponding Ueling-Serber potential in Eq. (11) can be written as follows:

$$\Phi_U(r) = -\frac{2\alpha}{3\pi r} \int_1^\infty dt \exp(-2rt/\alpha Z) \cdot \left(1 + \frac{1}{2t^2}\right) \frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r} C(x) \quad (14)$$

where $x = r/\alpha Z$. The quite complex expressions for determination of the electric and magnetic form-factors are given in ref. [15]. An account of the finite nuclear size effect changes (12) as follows [13,16]:

$$\Phi_U^{FS}(r) = -\frac{2\alpha^2}{3\pi} \int d^3r' \int_m^\infty dt \exp(-2t|r-r'|/\alpha Z) \cdot \left(1 + \frac{1}{2t^2}\right) \frac{\sqrt{t^2-1}}{t^2} \frac{\rho(r')}{|r-r'|}, \quad (15)$$

The next step is an account of the electron screening effect. It should be noted that the electron shells are not survived in the light pionic atoms during the cascade processes accompanying the formation of a pionic atom. However, in a case of the heavy systems, the internal electron shells survive and this fact should be reflected in a precise theory. Our procedure for accounting this effect is a standard one and includes addition to the total interaction potential SCF potential of the electrons, which can be determined within the Dirac-Fock method by solution of the standard relativistic Dirac equations. To realize this step, we have used the QED perturbation theory formalism for relativistic many-electron atom. Further in order to calculate probabilities of the Radiative transitions between energy level of the pionic atoms we have used the relativistic energy approach [16].

The final topic of the theory is calculation of the hyperfine structure parameters. Here one could use the standard theory of hyperfine structure of the usual multi-electron atom. As usually, the hyperfine structure is arisen because of the interaction of the orbital pion with a magnetic di-

pole moment m and quadruple electric moment Q of a nucleus. Hitherto, only magnetic contribution has been studied. The quadruple interaction is not treated hitherto. One could consider energy of the hyperfine interaction, which looks as:

$$W = W_\mu + W_Q = -\mu \cdot H(0) + \frac{1}{6} e \sum_{\alpha\beta} Q_{\alpha\beta} \frac{\partial^2 \phi}{\partial x_\alpha \partial x_\beta} \quad (15)$$

Here H and ϕ are defined as, respectively, the magnetic field and electrostatic potential produced by an electron (pion) in the position of the nucleus. Following to the standard procedure, after multiple transformations the final expression for the energy of the hyperfine splitting (magnetic part of) the energy levels of the atom in the pion:

$$E_1^{nIF} = \frac{\mu_I \mu_N e \mu_0 \hbar c^2}{4\pi (E_0^{nI} - \langle nl|V_0(r)|nl \rangle)} \times \left[\frac{F(F+1) - I(I+1) - l(l+1)}{2I} \right] \langle nl|r^{-3}|nl \rangle \quad (16)$$

Here

$$\mu_N = e\hbar / 2m_p c$$

and other notations are standard.

In a consistent precise theory it is important allowance for the contribution to the energy of the hyperfine splitting of the levels in the spectrum of the pion atom due to the interaction of the orbital momentum of the pion with the quadrupole moment of the atomic nucleus. The corresponding part looks as follows:

$$\langle LIFM|W_Q|LIFM \rangle \approx \Delta + BC(C+1) \quad (17)$$

where

$$C = F(F+1) - L(L+1) - I(I+1), \quad (18)$$

$$B = -\frac{3}{4} \frac{e^2 Q}{I(2I-1)} \frac{(\gamma \cdot L \|\eta_2\| \gamma \cdot L)}{\sqrt{L(L+1)(2L-1)(2L+1)(2L+3)}}, \quad (19)$$

$$\Delta = \frac{e^2 Q(I+1)}{(2I-1)} \frac{(\gamma \cdot L \|\mu_2\| \gamma \cdot L)L(L+1)}{\sqrt{L(L+1)(2L-1)(2L+1)(2L+3)}}. \quad (20)$$

Here L – is orbital moment of pion, F is a total moment of an atom.

3. Results and conclusions

Table 1 and Figure 1 shows the experimental data by Schröder et al, Gotta et al («Pionic hydrogen & pion mass collaboration»; Inst-PSI, Switzerland) and theoretical results: our data and data from other theories (KGF theory with analytical formula for the pionic H atom taking into account QED account within expansions in aZ by Schlessler-Indelicato, Schröder et al, two-channel theory considering the Uehling-Serber correction and the finite size of the nucleus by Sigg et al [4-12]. Besides, the QED contributions to the energy of the ground state pionic hydrogen are listed.

Table 1. **Theoretical (T), experimental (Exp) energies (eV) for the np-1s (n = 2-4) transitions in p-H and QED contributions to the ground state energy**

Data/ Transition	QED (meV)	2p-1s	3p-1s	4p-1s
T.:Schlessler- Indelicato	3238.287	2429.547	2878.844	3036.098
T.:Sigg et al	-	-	2878.808	3036.073
T.: Schroder et al	3238.264	-	2878.809	-
T.: Lyubovitski- Ruseitsky	3238.250	-	-	-

Our theory: ΔE_{EM}	3238.282	2429.546	2878.839	3036.098
Exp. (Schröder etal)	-	-	2885.916	-
Exp. (Gotta etal)	-	-	2885.929	-

Overall, between different theories is a good agreement that, in principle, due apparently

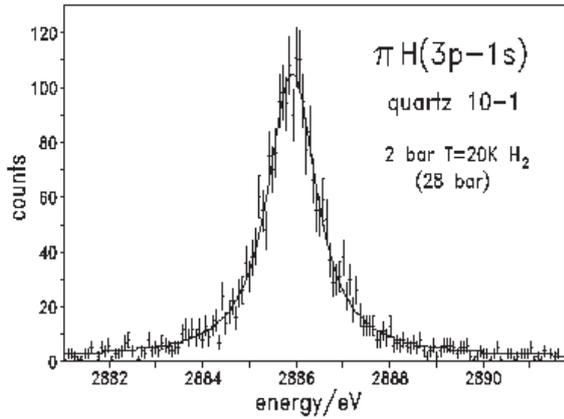


Fig 1. X-ray 3-1 transition in the spectrum of pionic H (Gotta etal); (narrow structure inside line indicates resolution spectrometer)

negligible contribution to QED, nuclear and others corrections for little Z (here $Z=1$, $aZ < 1$).

The pion-nuclear strong shift of the 1s level in pionic hydrogen DE_{1s} can be calculated as a difference between the experimental energy and exact electromagnetic value.

The corresponding results are listed below [4-12]: in the theory Schlessor-Indelicato etal with using the experimental data by Schröder etal: $DE_{1s} = -7.072 \pm 0.013$ (stat.) ± 0.034 (syst.) eV, with experimental data by Gotta etal: $DE_{1s} = -7.085 \pm 0.011$ (stat.) ± 0.026 (syst.); the result by Sigg

etal: $DE_{1s} = -7.108 \pm 0.013$ (stat.) ± 0.034 (syst.); the result by Gotta etal $DE_{1s} = 7.120 \pm 0.014$ eV; the theory of quantum defect by Mitroy-Ivallov gives the value: $DE_{1s} = 7.108 \pm 0.047$ eV.

Our relativistic theory provides such results: $DE_{1s} = 7.077 \pm \pm 0.013$ (stat.) ± 0.034 (syst.) with using the experimental data by Schröder etal and $DE_{1s} = 7.090 \pm 0.011$ (stat.) ± 0.026 (syst.) with the data by Gotta etal.

In table 2 we present our data on the hyperfine splitting energies of the 9p level ($F=1/2, 3/2$) for a number of the light, medium, heavy pionic atoms. The data by Trassinelli-Indelicato [6] are presented for comparison too.

Table 2. **Hyperfine splitting energies of the 9p level ($F=1/2, 3/2$) for a number of the light, medium, heavy pionic atoms: Theory I - Trassinelli-Indelicato ; Theory II – our data;**

Atom	Z	T.I	T.II
^1H	1	0.0001	0.0001
^{13}C	6	0.0060	0.0058
^{14}N	7	-	0.0296
^{15}N	7	-0.0039	-0.0033
^{17}O	8	-	0.0531
^{19}F	9	0.0767	0.0764
^{20}Ne	10	-	0.1003
^{43}Ca	20	-	-0.1256
^{57}Fe	26	0.0643	0.0639
^{129}Xe	54	-4.1295	-4.1620
^{133}Cs	55	-	1.0569
^{175}Lu	71	-	1.2304
^{181}Ta	73	-	1.2521
^{205}Tl	81	-	7.0407
^{202}Pb	82	-7.8662	-7.7954
^{235}U	92	-	9.2074

In table 3 we present our data on the different contributions to the 5f - 4d energy in pionic nitrogen (our data).

Table 3. **Different contributions to the 5f - 4d energy (eV)in pionic nitrogen (our data)**

Contribution	5f-4d
Coulomb	4054.7160
Finite size of a nucleus	0.0000
Self-energy	-0.0003
Vacuum polarization-Uehling-Serber	2.9462
Vacuum polarization-Wichman-Kroll	-0.0012
Vacuum polarization- Kallen-Sabry	0.0271
Relativistic recoil effect	0.0028
Other	-0.0020
Total energy	4057.6886

It is interesting to compare the results of our theory for the nitrogen atom with similar data in the theory of Trassinelli-Indelicato for the 5g-4f transition. The Radiative vacuum polarization corrections in our theory are as follows: the Uehling-Serber contribution -1.2478 eV; the total vacuum polarization one is 1.2618 eV; the total polarization contribution in the theory by Trassinelli-Indelicato: 1.2602 eV [6]. There is a very good agreement between two theories for sufficiently light atom of nitrogen. This is regarding the 5g-4f transition energies: our theory - 4055.3791eV, theory by Trassinelli-Indelicato: 4055.3801eV.

We have carried out the calculating the parameters (table 4) of a number of the X-ray transitions (5g-4f, 4f-3d) spectra of medium and heavy pionic atoms (^{43}Ca , ^{133}Cs , ^{175}Lu , ^{181}Ta , ^{205}Tl etc) with precise accounting of the relativistic, QED (corrections of the Uehling-Serber, Källen-Sabry, Wichmann-Kroll etc.), nuclear (finite size of the nucleus within the Fermi and Gauss models), electron screening (availability of the internal electronic shells) effects.

Table 4. **The 4f-3d, 5g-4f transition energies (keV) in spectra of some atoms (see text)**

Atom	Atom	E_{EXP} Berkley	E_{EXP} CERN	$E_{KGF+\alpha Z}$	E_{EM}	E_N^1	E_N^2
^{43}Ca	4f-3d	72.352 $\pm 0,009$	-	72.361	72.356	-	-
^{133}Cs	4f-3d	560.5 ± 1.1	562.0 ± 1.5	556.45	556.484	561.47	562.12
^{205}Tl	4f-3d	-	-	-	963.920	-	-
^{175}Lu	5g-4f	-	-	-	427.313	-	-
^{205}Tl	5g-4f	-	561.67 ± 0.25	559.65	559.681	560.93	561.63
^{202}Pb	5g-4f	-	575.56 ± 0.25	573.83	573.862	575.21	575.78
^{238}U	5g-4f	731.4 ± 1.1	732.0 ± 0.4	725.52	725.574	729.80	730.52

Note: $E_{EXP}(\text{Virginia})^{238}\text{U}$ (5g-f)=730.88 \pm 0.75

Our new data (E_{EM}) for a number of pionic atoms are listed in Table 4, where for comparison there are presented other experimental data (E_{EXP} ; Berkley, CERN, Virginia laboratories) and theoretical data: the KGF alternative theory of the use of model of the uniformly charged ball and αZ QED expansion decay ($E_{KGF+\alpha Z}$) [1-13]. Besides, we also list the corresponding data, obtained within different nuclear model calculations with the standard (E_N^1) and generalized (E_N^2) potentials [3-5,13].

Table 5 gives very interesting illustration of the electron screening contributions to the energy transitions 5g-4f, 4f-3d for the pion lead atom due to the presence of 2 [He], 4 [Be] and 10 [Ne] electrons, as well as (for Be-like configuration) contribution due to electron correlations.

Table 5. Contribution to the energy (eV) of the transition to a pion atom Pb, due to the presence of 2 [He], 4 [Be] and 10 [Ne] electron (our theory)

Transition	[He]	[Be]	[Be] ⁺ correlations	[Ne]
4-3	-56.15	-65.24	-65.16	-68.12
5-4	-63.08	-72.17	-72.08	-75.64

Our main conclusion is that an accounting of the Radiative, nuclear and electron-screening effects is very important in a precise relativistic theory of spectra of the pionic atoms. As example let us give the corresponding values of corrections: corrections to the energy, in particular, for the 5g-4f transition of atoms ⁴³Ca, ¹³³Cs, ¹⁷⁵Lu (5g-4f, 4f-3d), ¹⁸¹Ta, ²⁰⁵Tl (4f-3d), ²⁰²Pb, ²³⁸U, due to the radiative effects at $\sim 2-4.6$ keV, the nuclear effects - up to 0.2 keV and electron-screening effect, for example, for the 5g-4f, 4f-3d in the pionic Pb and others to availability of the 2[He]-10[Ne] electrons - $\sim 0.05-0.08$ keV. Using these measurements in the laboratories of CERN, Berkley, Virginia, one could obtain the pion-nuclear strong interaction shift (the difference between the experimental value and the “exact” electromagnetic energy), which are for the studied atoms lying in the limits $\sim 0.1-6.4$ keV.

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Abstract

A new theoretical approach to the description of spectral parameters pionic atoms in the excited states with precise accounting relativistic, radiation, nuclear, electron screening effects on the basis of the relativistic Klein-Gordon-Fock equation and QED perturbation theory formalism is developed. A consistent relativistic theory of hyperfine structure of spectra for the pionic atoms is presented. Numerical data on the electromagnetic contributions to the transition energies in spectra of different pionic atoms are listed.

Keywords: relativistic theory, hyperfine structure, pionic atoms

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РЕЛЯТИВИСТСКАЯ ТЕОРИЯ СПЕКТРОВ ПИОННЫХ АТОМОВ С УЧЕТОМ РАДИАЦИОННЫХ И ЯДЕРНЫХ ПОПРАВOK

Резюме

Предложен новый теоретический подход к описанию спектральных параметров пионных атомов в возбужденном состоянии с прецизионным учетом релятивистских, радиационных, ядерных и электронно-экранировочных эффектов на основе уравнения Клейна-Гордона-Фока и КЭД теории возмущений. Развита последовательная релятивистская теория сверхтонкой структуры пионных атомов. Приведены численные данные по электромагнитным вкладам в энергии переходов в спектрах различных пионных атомов.

Ключевые слова: релятивистская теория, сверхтонкая структура, пионные атомы

РЕЛЯТИВІСТСЬКА ТЕОРІЯ СПЕКТРІВ ПІОННИХ АТОМІВ З УРАХУВАННЯМ РАДІАЦІЙНИХ ТА ЯДЕРНИХ ПОПРАВОК

Резюме

Запропоновано новий теоретичний підхід до опису спектральних параметрів піонних атомів у збудженому стані з точною деталлю урахуванням релятивістських, радіаційних, ядерних та електронно-екраніровочних ефектів на основі рівняння Клейна-Гордона-Фока і КЕД теорії збурень. Розвинена послідовна релятивістська теорія надтонкої структури піонних атомів. Наведені чисельні дані по електромагнітним внескам в енергії переходів у спектрах різних піонних атомів.

Ключові слова: релятивістська теорія, надтонка структура, піонні атоми