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Computational studying energy and spectral parameters of hadronic (pionic) atoms with account of the strong pion-nuclear interaction

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Abstract. A relativistic computational approach to studying the energy and spectral characteristics of hadronic (pionic) atoms is presented and based on the Klein-Gordon-Fock equation with optimized π^--N interaction optical potential and relativistic many-body perturbation theory with correct treating radiation, electron-screening, nuclear effects. It is presented an effective scheme to computing energy levels shifts and widths, provided by a strong π^--N interaction and the interaction of the pion with QED vacuum (radiation width). It is based on using the model optimized optical complex π^--N interaction potential and relativistic energy approach with complex relativistic interparticle interaction potential. Data on the energy and spectral parameters for the pionic atom of ^{181}Ta are listed and compared with available experimental and alternative theoretical results.

1. Introduction

Studying the energy, spectral, radiative characteristics for exotic (hadronic, kaonic, pionic) atomic systems attracts a great interest as these atoms enable to probe different aspects of atomic and nuclear structure [1-10]. The knowledge of the corresponding properties for hadronic atomic systems can be used as a powerful tool for the study of particles and fundamental (for example, strong) interaction properties. It is worth to note that one of the most sensitive tests for the chiral symmetry breaking scenario in the modern nuclear physics is provided by investigation of the exotic hadronic atomic systems. These facts explain intense theoretical and experimental works on exotic atoms in different laboratories (CERN, Japan, Berkley, Virginia etc). Nowadays the transition energies in pionic (kaonic, muonic etc) atomic systems can be measured with an unprecedented precision. It allows to study the strong interaction at low energies measuring the energy and natural width of the ground level with a precision of few meV. There are a few theoretical approaches to studying spectra and spectral properties of the exotic (pionic, kaonic, muonic etc) atomic systems (see details in Refs. [1-55]). The most difficult aspects of the theoretical modelling are connected with the accurate treatment of the pion-nuclear strong interaction as the electromagnetic part of the problem can be in principle reasonably accounted for. In Refs. [2] it has been presented an effective relativistic approach to studying the energy and spectral characteristics of heavy hadronic (pionic) atoms. It is based on the Klein-Gordon-Fock equation with optimized π^--N interaction optical potential and relativistic many-body perturbation theory with correct accounting for the radiation, electron-screening, nuclear effects effects [31,32]. It has been developed an effective theory for calculating energy levels shifts and widths, provided by a strong π^--N interaction ("strong" width) and the interaction of the pion with

QED vacuum (radiation width) within the model optimized optical complex π^--N interaction potential and relativistic energy approach based on the Gell-Mann and Low formalism with complex relativistic interparticle interaction potential [56-68]. Here we apply it to computing the energy and spectral parameters of the pionic ^{181}Ta atom. The obtained theoretical data are listed and compared with available experimental and other theoretical results. All calculations are performed with using the modified blocks [2] of the PC computational code "Superatom-ISAN" (see details in Refs. [60-88]).

2. The theoretical method

2.1. The Klein-Gordon-Fock equation and electromagnetic interaction potentials

The relativistic electron wave functions are determined from solution of the Klein-Gordon-Fock equation (pion is the Boson with spin 0, mass: m_{π^-}=139.57018 MeV, r_{π^-}=0.672±0.08 fm) with a general potential (the latter includes an electric and polarization potentials of a nucleus plus the strong pion-nuclear interaction potential):

$$\{\frac{1}{c^2}[E+eV_0(r)]^2+\hbar^2\nabla^2-m^2c^2\}\varphi(x)=0\,. \tag{1}$$

Here E is the total energy of the system (sum of the mass energy mc^2 and binding energy ε_0). The central potential V_0 is the sum of the electric potential of a nucleus, vacuum-polarization potential and the strong interaction potential. As usually (see [2,31,32], the nuclear potential for the spherically symmetric density (as the first approximation) $\rho(r|R)$ can be presented as follows:

$$V_{nucl}(r|R)=-(1/r)\int_0^r dr'r'^2\rho(r'|R)+\int_r^\infty dr'r'\rho(r'|R)\cdot \tag{2}$$

Probably nowadays the most consistent approach to determination of $\rho(r|R)$ is in using the relativistic mean-field (RMF) model, which has been designed as a renormalizable meson-field theory for nuclear matter and finite nuclei. However, quite physically reasonable acceptable approximation is given by the known Gauss or Fermi nuclear models. In particular, the density can be approximated by the Fermi function:

$$\rho(r)=\rho_0/\{1+\exp[(r-c)/a)]\}\,, \tag{3}$$

where the parameter a=0.523 fm, the parameter c is chosen in such a way that it is true the following condition for average-squared radius: $<r^2>^{1/2}=(0.836\cdot A^{1/3}+0.5700)$fm. The effective computational algorithm for definition of the potential $V_{nucl}(r|R)$ is based on the known Ivanov-Ivanova et al [56] method of differential equations (see Refs. [2-4,31,32]). It allows to determine the nuclear potential by solution of the differential equations system (the Fermi model):

$$V'nucl(r,R)=(1/r^2)\int_0^r dr'r'^2\rho(r',R)\equiv(1/r^2)y(r,R),\quad y'(r,R)=r^2\rho(r,R), \tag{4}$$

$$\rho'(r)=(\rho_0/a)\exp[(r-c)/a]\{1+\exp[(r-c)/a)]\}^2 \tag{5}$$

with the corresponding boundary conditions.

The next important theoretical step is a consistent and accurate accounting for the QED effects in computing the energy parameters of pionic atoms. To take into account the radiation (QED) corrections, namely, the important effect of the vacuum polarization one could use the procedure, which is in details described in the Refs. [3,4]. The important radiation contributions are given by the standard Uehling-Serber term and the Källen-Sabry and Wichmann-Kroll corrections of higher orders

(such as $[\alpha\,(Z\alpha)]^n$ (n=2,..), $\alpha^2(\alpha Z)$, $\alpha\,(Z\alpha)^n$ (n=3) etc; α being the fine structure constant). In order to take into consideration an effect of the vacuum polarization in the first perturbation theory order one should use the generalized Uehling-Serber potential with modification to account for the high-order radiative corrections. It can be written as follows:

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt \exp\left(-2rt/\alpha Z\right)\left(1+1/2t^2\right)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \tag{6}$$

where $g=r/(\alpha Z)$. More correct and consistent approach is presented in Refs. [42,43,52-62]. An accounting of the nuclear finite size effect modifies the potential (6) as follows:

$$U^{FS}(r) = -\frac{2\alpha^2}{3\pi}\int d^3r'\int_m^\infty dt \exp\left(-2t|r-r'|/\alpha Z\right)\times\left(1+\frac{1}{2t^2}\right)\frac{\sqrt{t^2-1}}{t^2}\frac{\rho(r')}{|r-r'|}, \tag{7}$$

According to Refs. [3], the modified Uehling-Serber potential can be determined as a quadrature (7) and approximated with high precision by a simple analytical function. The use of new approximation of the Uehling potential permits one to decrease the calculation errors for this term down to 0.5 – 1%. A method for calculation of the self-energy part of the Lamb shift is based on an idea by Ivanov-Ivanova [58], which generalizes the known hydrogen-like method by Mohr and radiation model potential method by Flambaum-Ginges (look details in Refs. [46-50]).

2.2. Strong pion-nuclear interactions in pionic atomic system

The most difficult aspect of the theoretical study of pionic atomic systems is connected with a consistent and adequate account for the strong pion-nuclear interaction. Naturally, the most fundamental and exact microscopic theory of the strong interactions is provided by the modern quantum chromodynamics. Usually, one can consider the regimes of relatively low and high energies (asymptotic freedom) in physics of pionic systems. In a case of the low energies so called coupling constant increases to the order 1 and, therefore, this perturbation methods fail to describe the interaction of strongly interacting hadrons. At present time there are different approaches to treating pion-nuclear interaction even at relatively low energies (look details in Refs. [1,2,10,23-28,33-44]). From the computational viewpoint a more simplified approach to treatment of the strong interaction in the pionic atomic system is provided by the optical potential model (c.g. [1,33]). The most popular version of this method is based on using the known generalized Ericson-Ericson potential:

$$V_{\pi^- N} = V_{opt}(r) = -\frac{4\pi}{2\overline{m}}\left\{q(r)\nabla\frac{\alpha(r)}{1+4/3\pi\xi\alpha(r)}\nabla\right\},$$

$$q(r) = \left(1+\frac{m_\pi}{m_N}\right)\left\{b_0\rho(r)+b_1\left[\rho_n(r)-\rho_p(r)\right]\right\}+\left(1+\frac{m_\pi}{2m_N}\right)\left\{B_0\rho^2(r)+B_1\rho(r)\delta\rho(r)\right\}, \tag{8}$$

$$\alpha(r) = \left(1+\frac{m_\pi}{m_N}\right)^{-1}\left\{c_0\rho(r)+c_1\left[\rho_n(r)-\rho_p(r)\right]\right\}+\left(1+\frac{m_\pi}{2m_N}\right)^{-1}\left\{C_0\rho^2(r)+C_1\rho(r)\delta\rho(r)\right\},$$

where $\rho_{p,n}(r)$ are distribution of density of the protons and neutrons, respectively, ξ is a parameter such that $\xi=0$ corresponds to the case of "no correlation" while $\xi=1$ in the case of accounting of anticorrelations between nucleons); the isoscalar and isovector parameters b_0, c_0, B_0, b_1,c_1, C_0 B_1, C_1 are corresponding to the s-wave and p-wave (repulsive and attracting potential member) scattering

length respectively in the combined spin-isospin space with taking into account for absorption of pions (with different channels for p-p pair $B_{0(pp)}$ and *p-n* pair $B_{0(pn)}$), the Lorentz-Lorentz effect in the p-wave interaction and isospin and spin dependence of an amplitude π-N scattering: $(b_0\rho(r) \to b_0\rho(r) + b_1\{\rho_p(r) - \rho_n(r)\}$ [2]).

2.3 *Complex energy of pionic atomic system*

The energy of a multielectron hadronic atom can be represented as follows:

$$E \approx E_{KG} + E_{FS} + E_{VP} + E_N; \tag{9}$$

Here E_{KG} -is the energy of a pion in a nucleus (Z, A) with the point-like charge (dominative contribution in (9)), E_{FS} is the contribution due to the nucleus finite size effect, E_{VP} is the radiation correction due to the vacuum-polarization effect, E_N is the energy shift due to the strong interaction V_N. The strong pion-nucleus interaction contribution into energy can be directly found from the solution of the Klein-Gordon-Fock equation with the corresponding pion-nucleon potential, for example, in the optical potential approximation (8). Since the corresponding optical potential contains complex parameters, the relevant energy eigen-values of the Klein-Gordon-Fock equation for the definite state $(i = nl)$ are complex valued too:

$$E_i = \mathrm{Re}\, E_i + i\, \mathrm{Im}\, E_i = \mathrm{Re}\, E_i - (i/2)\Gamma_i, \tag{10}$$

where Γ_i is a width of pionic energy level, which is determined by the imaginary part of (10). The total width of any level is determined as by the strong pion-nuclear interaction contribution Γ_i^s (pion absorption) as by the electromagnetic contribution Γ_i^{rad}. The latter is determined by a probability of the electromagnetic radiation transition (including the Auger process probability Γ_i^A) on the lower level. In order to calculate electromagnetic interaction characteristics (for example, probabilities of transitions in spectrum of the pionic atom) we have implemented the known (in a theory of usual multi-electron atom) relativistic energy formalism [56-68]. In this approach (an energy of any excited state being a complex quantity) a shift of the total energy level is usually represented as:

$$\Delta E_i = \mathrm{Re}\,\Delta E_i + i\,\mathrm{Im}\,\Delta E_i = \mathrm{Re}\,\Delta E_i - (i/2)\Gamma_i^{rad}, \tag{11}$$

where Γ_i^{rad} is a radiation width, and the corresponding radiative transition probability in the usual atomic system P~Γ_i^{rad}. In order to compute the latter we use the generalized relativistic energy approach. It is worth to remind that an initial general energy formalism combined with an empirical model potential method in a theory of atoms and multicharged ions has been developed by Ivanov-Ivanova et al [57-62]; further more general ab initio gauge-invariant version of relativistic energy approach has been presented by Glushkov-Ivanov [65-67]. The latter has been used in this work.

3. The results and conclusions

In Table 1 we list the values of the optical potential parameters, which have been used in our and other calculations [34-44,2]. It is worth to explain the used classification and abbreviations of the corresponding sets of optical potential parameters: Tauscher, ξ=0 – Tau1; Tauscher, ξ=1 – Tau2; Batty et al – Bat; Seki et al – Sek; Nagels – Nag; de Laat-Konijin et al – Laat, this theory - Odes [2,33-44]. Usually the potential parameters were initially obtained by calibration of the experimental data on pion-nuclear scattering for the light and medium nuclei. Further application of the model to the heavy systems and relatively low-lying states showed imperfections (in some cases) of these sets of the parameter values (the known pion anomalies). For example, experimental (low-energy scattering of pions; LAMPF) results for relatively low-lying states of pion at levels 3d, 2p, 1s (in such heavy atoms

as Ta, Bi et al) have shown that the appropriate values of width due to strong interaction a factor two and more are lower than the values specified within the optical potential model using the earliest parameterization [1,33-35]. Under the parameterization of the optical potential authors [41,43] left without changing the parameters settings that are the most reliably identified, namely: ReB_0, ImB_0, c_0, c_1, ReC_0 , ImC_0. At the same time the parameters whose values differ most strongly in different sets, in particular, b_1 (plus parameters, which are usually not included so far in the basic optical potential parameterizations, i.e. ImB_1, ImC_1), should be optimized. This is achieved by receiving preliminary calculated relationships for the energy shifts and widths (for a number of states of the following systems: ^{20}Ne, ^{133}Cs, ^{208}Pb) upon the b_1, ImB_1, ImC_1 parameter values. As illustration In Table 2 we list the dependences of shifts and widths for the 4f, 3d levels due to the strong pion nuclear interaction upon the parameter ImB_1 value for the pionic ^{181}Ta.

Table 1. The values of the optical potential parameters, used in different calculations (see text).

	Tauscher ξ=0 [34]	Tauscher ξ=1 [34]	Batty ξ=1 [35]	Seki ξ=1 [36]	Nagels ξ=1[40]	Row78 ξ=1[37]	Laat ξ=1 [43,44]	Odes ξ=1 [2]	
b_0	-0.0296	-0.0293	-0.017	0.003	-0.013	-0.004	0.007	0.003	m_π^{-1}
b_1	-0.077	-0.078	-0.13	-0.143	-0.092	-0.094	-0.075	-0.094	m_π^{-1}
ReB_0	0	0	-0.0475	-0.15	-	-	-0.18	-0.15	m_π^{-4}
ImB_0	0.0436	0.0428	0.0475	0.046	-	-	0.058	0.046	m_π^{-4}
c_0	0.172	0.227	0.255	0.21	0.209	0.23	0.266	0.21	m_π^{-3}
c_1	0.22	0.18	0.17	0.18	0.177	0.17	0.40	0.18	m_π^{-3}
ReC_0	-	-	-	0.11	-	-	0.07	0.11	m_π^{-6}
ImC_1	-	-	-	-	-	-	-0.34	-0.25	m_π^{-6}

Table 2. The dependence of shifts and widths for the 4f, 3d levels due to the strong pion nuclear interaction upon the parameter ImB_1 value for ^{181}Ta

ImB_1	ε_0^{4f} (^{181}Ta)	Γ_0^{4f} (^{181}Ta)	ε_0^{3d} (^{181}Ta)	Γ_0^{3d} (^{181}Ta)
0.00	0.508	0.41	13.5	34.9
0.02	0.517	0.39	14.1	30.8
0.04	0.525	0.37	14.7	27.5
0.06	0.533	0.35	15.2	24.8
0.08	0.543	0.33	15.8	22.6
0.10	0.554	0.30	16.3	20.3
0.12	0.566	0.28	16.8	18.3
Exp.	0.56±0.04	0.31±0.05	16.2±1.3	20.1±1.5

In Table 3 we list our calculated (the relativistic Klein-Gordon-Fock theory combined with energy approach) data on the3d, 4f, 5g levels radiation widths for π^--Ta atom. There are also listed the analogous data by Laat et al [43,44], obtained using the relativistic Klein-Gordon-Fock model and Hartree-Fock approximation. In Table 4 we list theoretical and experimental data (in keV) for 4f, 3d levels shift and width due to strong π-N interaction [2,34-44]. In our parameterization of a strong potential the most reliably defined (B_0, c_0, c_1, C_0) parameters are remained unchanged. The parameters whose values differ greatly in different sets, in particular, b_1 (b_1 = -0.094) plus still not included ones ImB_1, ImC_1 have been optimized by computing dependency of the strong shift on the parameters b_1, ImB_1,ImC_1 for number of π^--atoms.

Table 3. The radiation widths of the 3d, 4f, 5g levels in some π^-A systems

Nucleus	Γ^1_{rad}(5g) [43]	Γ^2_{rad} (5g) This work	Γ^1_{rad} (4f) [43,44]	Γ^2_{rad} (4f) This work	Γ^1_{rad} (3d) [43,44]	Γ^2_{rad} (3d) This work
^{181}Ta	25.7	23.5	90.9	88.6	369.9	366.1

Table 4. Theoretical and experimental data for the 4f, 3d levels shift and widths (keV) provided by the strong pion-nuclear interaction for the π^- -^{181}Ta atomic system (see text)

4f	Exp	H-like Func.	Tau1 ξ=0	Tau2 ξ=1	Bat ξ=1	Sek ξ=1	Laat ξ=1	Our ξ=1
ε_{4f}	0.56±0.04	0.47	0.57	0.54	0.53	0.47	0.60	0.55
Γ_{4f}	0.31±0.05	0.16	0.31	0.30	0.31	0.27	0.31	0.31
ε_{3d}	16.2±1.3	-	19.6	16.4	10.4	4.4	14.4	16.1
Γ_{3d}	20,1±1,5	-	40,5	37,5	33,4	26,2	27,6	20.2

In Table 5 data on the *4f-3d, 5g-4f* transition energies for pionic atoms ^{181}Ta are presented. There are also listed the measured values of the Berkley, CERN and Virginia laboratories and alternative data obtained on the basis of computing within alternative versions of the Klein-Gordon-Fock (KGF) theory with taking into account for a finite size of the nucleus in the model uniformly charged sphere and the standard Uehling-Serber radiation correction (see [1,2,4,23] and Refs. therein).

Table 5. Transition energies (keV) in the spectra of π-^{181}Ta atom (see text)

Trans.	Berkley E_{EXP}	CERN E_{EXP}	E_{KGF+EM} [1, 4]	E_{KGF-EM} [23]	E_N [4,23]	E_N, This work
5g-4f	453.1±0.4	453.90±0.20	453.06	453.78	453.52 453.62	453.71
4f-3d	-	1008.4±1.3	-	-	992.75	1008.80

To conclude, let us note that the key factors of the acceptable agreement between experimental and theoretical data for complex pionic atoms are provided by a correct treatment of the nuclear, relativistic, radiative and inter-electron correlation corrections. Using different schemes for accounting of these correlations explains a difference between calculational data, obtained within the Klein-Gordon-Fock approach. The further refinement of the obtained data can be reached by means of accounting for such effects as a spatial distribution of the magnetic moment inside a nucleus, nuclear-polarization corrections etc.

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