An advanced relativistic approach is presented to studying spectroscopy and photodynamics of the exotic (pionic) atomic systems based on the Klein-Gordon-Fock equation approach and relativistic many-body perturbation theory with accounting for the fundamental electromagnetic and strong pion-nuclear interactions. The strong pion-nuclear interactions are taken into account by means of using the generalized strong pion-nuclear optical potential model with the effective Ericson-Ericson potential. The nuclear finite size effect is taken into consideration within the Fermi model. In order to take the nuclear quadrupole deformation effects on pionic processes into account we have used the model by Toki et al. The radiative corrections are effectively taken into account within the generalized Uehling-Serber approximation to treat the Lamb shift vacuum polarization part. The advanced data for the energy and spectral parameters for pionic atoms of the $^{173}$Yb, $^{175}$Lu, $^{197}$Au, $^{208}$Pb, $^{238}$U with accounting for the radiation (vacuum polarization), nuclear (finite size of a nucleus ) and the strong pion-nuclear interaction corrections are listed.

1. Introduction

Our work is devoted to the further development of the relativistic theoretical approach [1-3] to the description of spectra and different spectral parameters, in particular, radiative transitions probabilities for hadronic (pionic) atoms in the excited states with precise accounting for the relativistic, nuclear and radiative effects.

Here we present an advanced relativistic theory of spectra of the exotic (pionic) atomic systems based on the Klein-Gordon-Fock equation approach and relativistic many-body perturbation theory with accounting for the fundamental electromagnetic and strong pion-nuclear interactions. The latter has been performed by means of using the advanced strong pion-nuclear optical potential model with the generalized Ericson-Ericson potential. The nuclear finite size effect is taken into consideration within the Fermi model. In order to take the nuclear quadrupole deformation effects on pionic processes into account we have used the model by Toki et al. The radiative corrections are effectively taken into account within the generalized Uehling-Serber approximation to treat the Lamb shift vacuum polarization part. In order to take the contribution of the Lamb shift self-energy part into account we have used the generalized non-perturbative procedure, which generalizes the Mohr procedure and radiation model potential method by Flambaum-Ginges. The results of calculation of the energy and spectral parameters for pionic atoms of the $^{173}$Yb, $^{175}$Lu, $^{197}$Au, $^{208}$Pb, $^{238}$U with accounting for the radiation (vacuum polarization), nuclear (finite size of a nucleus ) and the strong pion-nuclear interaction corrections are presented.

As it is well known [1-22] spectroscopy of hadronic atoms already in the electromagnetic sector is extremely valuable area of research that provide unique data for different areas of physics, including nuclear, atomic, molecular physics, physics of particles, sensor electronic etc. While determining the properties of pion atoms in theory is very simple as a series of H such models and more sophisticated methods such combination chiral perturbation theory (PT), adequate quantitative description of the spectral properties of atoms in the electromagnetic pion sector (not to mention even the strong interaction sector ) requires the development of High-precision approaches,
which allow you to accurately describe the role of relativistic, nuclear, radiation QED (primarily polarization electron-positron vacuum, etc.). pion effects in the spectroscopy of atoms.

The most popular theoretical models for pionic and kaonic atoms are naturally based on the using the Klein-Gordon-Fock equation, but there are many important problems connected with accurate accounting for as pion-kaon-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 [1-23]). A development of the comprehensive theory of computing energy, spectral and radiation characteristics is of a great interest and importance in a modern theory of the hadronic atom spectra too [1-36].

2. Relativistic Spectroscopy of pionic atomic systems

Here we present a brief description of the key moments of our approach (more details can be found in Refs. [1-3]). As a negative pion is the Boson with spin 0, mass: \( m_\pi = 139.57018 \) \( \text{MeV} \), \( r_\pi = 0.672 \pm 0.08 \) \( \text{fm} \), the relativistic particle wave functions are determined from solution of the Klein-Gordon-Fock equation with a general potential \( V_C \), which includes an electric and polarization potentials of a nucleus (plus the strong pion-nuclear interaction potential). Generally speaking, the Klein-Gordon-Fock equation can be rewritten as the corresponding two-component equation [1-3]:

\[
\mathcal{L} = \left( \sigma_3 + i \sigma_2 \right) \frac{\nabla^2}{2 \mu} + \sigma_3 \mu + \left( \sigma_3 + i \sigma_2 \right) V^{(0)}_{\text{pp}} + V_C^{(0)} \Psi = E_0 \Psi, \tag{1}
\]

where \( \sigma_i \) are the Pauli spin matrices and

\[
\Psi_i = \frac{1}{2} \left( \begin{array}{c}
1 + \left( E - V^{(0)}_C \right) / \mu \phi_i \\
n - \left( E - V^{(0)}_C \right) / \mu \phi_i
\end{array} \right). \tag{2}
\]

This equation is equivalent to the stationary Klein-Gordon-Fock equation. The corresponding non-stationary Klein-Gordon-Fock equation can be written in the following standard form:

\[
\mu^2 c^4 \Psi(x) = \frac{1}{c^2} \left[ \hbar \hat{c}^2 + eV_{\phi}(r) \right] - \hbar^2 \nabla^2 \Psi(x) \tag{3}
\]

where \( c \) is the speed of light, \( h \) is the Planck constant, \( J \) is the reduced mass of the pion-nuclear system, and \( \Psi_0(x) \) is the scalar wave function of the space-temporal coordinates. Usually one considers the central potential \( V_0(r) \), \( 0 \) approximation with the stationary solution:

\[
\Psi(x) = e^{-\left( E V_{\phi} / \hbar \right)} \phi(x), \tag{4}
\]

where \( \phi(x) \) is the solution of the stationary equation:

\[
\frac{1}{c^2} \left( E + eV_{\phi}(r) \right)^2 + \hbar^2 \nabla^2 - \mu^2 c^2 \phi = 0 \tag{5}
\]

Here \( E \) is the total energy of the system (sum of the mass energy \( mc^2 \) and binding energy \( \varepsilon_0 \)). In principle, the central potential \( V_0 \) is the sum of the following potentials: the electric potential of a nucleus, vacuum-polarization potential. The strong interaction potential can be added below.

Generally speaking, an energy of the pionic atomic system can be represented as the following sum:

\[
E \approx E_{K0} + E_{FS} + E_{QED} + E_N. \tag{6}
\]

where \( E_{K0} \) is the energy of a pion in a nucleus \( \{ Z, A \} \) with the point-like charge, \( E_{FS} \) is the contribution due to the nucleus finite size effect, \( E_{QED} \) is the radiation QED correction, \( E_N \) is the energy shift due to the strong interaction \( V_N \).

Further let us consider in details the radiation or QED effects since their consistent and accurate accounting for is of a great importance and interest in spectroscopy of the pionic atomic systems. In order to take the radiation (QED) corrections into account, namely, the important effect of the vacuum polarization, one could use the procedure, which is in details presented, for example, in the Refs. [21-24]. Figure 1 illustrates the Feynman diagrams, which describe QED effect of the vacuum polarization: A1 – the Uehling-Serber term; A2, A3 – terms of order.
\[ [a(Za) \square^n \ (n=2,..); \ A4 - \text{the Källen-Sabry correction of order } \alpha^n (Za); \ A5 - \text{the Wichmann-Kroll correction of order } \alpha^n (Za)^n \ (n=3). \]

Figure 1. The Feynman diagrams, which describe QED effect of the vacuum polarization: A1 – the Uehling-Serber term; A2, A3 – terms of order \([a(Za) \square^n \ (n=2,..); \ A4 - \text{the Källen-Sabry correction of order } \alpha^n (Za); \ A5 - \text{the Wichmann-Kroll correction of order } \alpha^n (Za)^n \ (n=3). \]

An effect of the vacuum polarization is usually considered in the first PT theory order by means of the generalized Uehling-Serber potential with modification to account for the high-order radiative corrections. In particular, the generalized Uehling-Serber potential can be written as follows:

\[
U(r) = -\frac{22\alpha Z^2}{3\pi r} \int_0^r dr' \frac{r'^2}{r} \exp(-2\alpha(aZ)^{1/2}) \left[ 1 - \frac{r'^2}{r} \right] = -\frac{22\alpha Z^2}{3\pi r} \zeta(a), \tag{7}
\]

where \(g = r/(aZ)\). More correct and consistent approach is presented in Refs. [21-24].

The vacuum-polarization block includes the radiation potential of the standard vacuum-polarization contribution of the Uehling-Serber, supplemented by the contributions due to the Källen-Sabry \([\sim \alpha^n (Za)\] order) and Wichmann-Kroll \([\sim \alpha^n (Za)^n] \) order) corrections. The nuclear potential for the spherically symmetric density \(\rho(r)\) can be presented as follows:

\[
V_{\text{nucl}}(r,R) = \left(1/r^2\right) \int_0^r dr' r'^2 \rho(r', R) \equiv \left(1/r^2\right) y(r, R)
\]

where \(y^2(r,R) = r^2 \rho(r, R)\), \(\rho^2(r) = \left(\rho_0/a\right) \exp(10)\).

\[
\rho(r) = \rho_0(r) + \sum_{k \geq 2} \frac{2k+1}{16\pi} \rho_k(r) Y_k^0(\hat{r}), \tag{11}
\]

where the quantity \(\rho_k(r)\) is defined as follows:

\[
\rho_k(r) = \left[ \int \frac{16\pi}{2k+1} \delta(r - r_i) Y_k^0(\hat{r}) \right] \langle JJ \rangle_{Y_k^0(\hat{r})}. \tag{12}
\]

One should consider the case \(k=2\), which corresponds to the nuclear quadrupole density. The Woods-Saxon-like form for the nuclear density distribution in the intrinsic frame is (see, e.g., [21]):

\[
\bar{\rho}(r) = \rho_n \left[ 1 + \exp \left( \frac{r - R(\theta)}{a} \right) \right], \tag{13}
\]

where

\[
R(\theta) = R \left[ 1 + \beta Y_2^0(\theta) \right], \tag{14}
\]

\(\rho_n\) is the normalization constant, \(\beta\) is a quadrupole deformation parameter.

\[ [a(Za) \square^n \ (n=2,..); \ A4 - \text{the Källen-Sabry correction of order } \alpha^n (Za); \ A5 - \text{the Wichmann-Kroll correction of order } \alpha^n (Za)^n \ (n=3). \]
Further in order to calculate probabilities of the radiative transitions between energy level of the pionic atoms we have used the well-known relativistic energy approach (c. g.[16-18,23-28, 36-39]).

More simplified and sufficiently popular approach to treating the strong interaction in the pionic atomic system is provided by the well known optical potential model (see, e.g., [4,10]). Recall that in the model of optical potential for the description of pion-nuclear interaction the potential

\[ V_{\pi N_{(opt)}} = \text{Re} V + i \text{Im} V \]  

is used. Dedicated, as a rule, separate s-wave and p-wave pion-nuclear scattering are derived in accordance with the repulsive and attracting parts of the optical potential. In order to describe the strong \( \pi N \) interaction we use the potential model where the generalized Ericson-Ericson potential is as follows [4]:

\[ V_{\pi N} = V_{opt}(r) = -\frac{4\pi}{2m} \left\{ q(r) V + \frac{\alpha(r)}{1+4/3\rho^{2}(r)} \right\}, \]  

(15)

\[ q(r) = \frac{1}{m_{\pi}} \left[ b_{0}\rho(r) + b_{1}\left[\rho_{p}(r) - \rho_{n}(r)\right] \right] + \frac{m_{n}}{2m_{p}} \left[ b_{0}\rho^{2}(r) + b_{1}\rho(r)\delta\rho(r) \right], \]  

(16a)

\[ \alpha(r) = \left(1 + \frac{m_{\pi}}{m_{N}}\right) \cdot \left[ C_{0}\rho^{2}(r) + C_{1}\rho(r)\delta\rho(r) \right], \]  

(16c)

Here \( \rho_{p,n}(r) \) – distribution of a density of the protons and neutrons, respectively, \( \xi \)–parameter (\( \xi = 0 \) corresponds to case of “no correlation”, \( \xi = 1 \), if there are anticorrelations between nucleons); respectively isoscalar and isovector parameters \( b_{0}, C_{0}, b_{1}, C_{1}, b_{2,1}, b_{2,1} \), \( C_{0}, B_{1}, B_{2} \), \( C_{1} \) – are corresponding to the s-wave and p-wave (repulsive and attracting potential member) scattering length in the combined spin-isospin space with taking into account the absorption of pions (with different channels for p-p pair \( B_{0}(pp) \) and p-n pair \( B_{0}(pn) \)), the Lorentz-Lorenz effect in the p-wave interaction and isospin and spin dependence of an amplitude \( \pi N \) scattering:

\[ b_{0}\rho(r) - b_{0}\rho(r) + b_{1}\left[\rho_{p}(r) - \rho_{n}(r)\right], \]  

(17)

The description of numerical values of the potential parameters is in details described in Refs. [1-4,10-152]. Other details are in Refs. [1-3,34-40].

3. Results and conclusions

In Table 1 the advanced data on the 4f-3d, 5g-4f transition energies for pionic atoms of the \( ^{173}\text{Yb}, ^{175}\text{Lu}, ^{197}\text{Au}, ^{208}\text{Pb}, ^{238}\text{U} \) 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 the finite size of the nucleus in the model uniformly charged sphere and the standard Uehling-Serber radiation correction [1-3,5,6, 14, 15, 34, 35].

<table>
<thead>
<tr>
<th>( \Delta A )</th>
<th>( E_{N} )</th>
<th>( E_{N} )</th>
<th>( E_{N} )</th>
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<tbody>
<tr>
<td>CERN</td>
<td>[5,6,14]</td>
<td>KGF+EM</td>
<td>KGF+EM</td>
</tr>
<tr>
<td>( ^{173}\text{Yb} ) 5g-4f</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( ^{179}\text{Au} ) 5g-4f</td>
<td>533.16 ± 0.20</td>
<td>532.5 ± 0.5</td>
<td>528.95</td>
</tr>
<tr>
<td>( ^{205}\text{Tl} ) 5g-4f</td>
<td>561.67 ± 0.25</td>
<td>559.65</td>
<td>559.681</td>
</tr>
<tr>
<td>( ^{208}\text{Pb} ) 5g-4f</td>
<td>575.56 ± 0.25</td>
<td>573.83</td>
<td>573.862</td>
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<tr>
<td>( ^{238}\text{U} ) 5g-4f</td>
<td>732.0 ± 0.4</td>
<td>731.4 ± 1.1</td>
<td>725.52</td>
</tr>
<tr>
<td>( ^{173}\text{Yb} ) 4f-3d</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( ^{179}\text{Au} ) 4f-3d</td>
<td>1187.3 ± 1.9</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( ^{208}\text{Pb} ) 4f-3d</td>
<td>1282 ± 2.2</td>
<td>-</td>
<td>-</td>
</tr>
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<td>730.92</td>
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<tr>
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<td>838.67</td>
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<td>-</td>
<td>-</td>
<td>923.14</td>
</tr>
<tr>
<td>( ^{208}\text{Pb} ) 4f-3d</td>
<td>-</td>
<td>-</td>
<td>1167.92</td>
</tr>
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</table>

Table 1. The 5g-4f and 4f-3d transition energies (keV) in the spectra of heavy pionic atoms (see text)
The analysis of the presented data confirms an importance of the consistent and correct accounting for the radiation (vacuum polarization) and the strong pion-nuclear interaction corrections. The contributions due to the nuclear finite size effect and electron screening correction should be accounted in a precise theory too. A correct treatment of the nuclear, relativistic, radiative and other effects could provide the physically reasonable agreement between experimental and theoretical data on the multi-electron pionic atoms.

References

17. Glushkov, A.V.; Ivanov, L.N. Radiation decay of atomic states: atomic residue polarization and gauge noninvariant


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SPECTROSCOPY AND DYNAMICS OF HEAVY EXOTIC PIONIC ATOMIC SYSTEMS: ADVANCED RELATIVISTIC THEORY

Summary. An advanced relativistic approach is presented to studying spectroscopy and photodynamics of the exotic (pionic) atomic systems based on the Klein-Gordon-Fock equation approach and relativistic many-body perturbation theory with accounting for the fundamental electromagnetic and strong pion-nuclear interactions. The strong pion-nuclear interactions are taken into account by means of using the generalized strong pion-nuclear optical potential model with the effective Ericson-Ericson potential. The nuclear finite size effect is taken into consideration within the Fermi model. In order to take the nuclear quadrupole deformation effects on pionic processes into account we have used the model by Toki et al. The radiative corrections are effectively taken into account within the generalized Uehling-Serber approximation to treat the Lamb shift vacuum polarization part. The advanced data for the energy and spectral parameters for pionic atoms of the \(^{173}\)Yb, \(^{175}\)Lu, \(^{197}\)Au, \(^{208}\)Pb, \(^{238}\)U with accounting for the radiation (vacuum polarization), nuclear (finite size of a nucleus ) and the strong pion-nuclear interaction corrections are listed.

Keywords: relativistic theory, pionic atomic systems, spectroscopy and photodynamics

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СПЕКТРОСКОПІЯ ТА ДИНАМІКА ВАЖКИХ ЕКЗОТИЧНИХ ПІОННИХ АТОМНИХ СИСТЕМ: УДОСКОНАЛЕНА РЕЛЯТИВІСТСЬКА ТЕОРІЯ

Резюме. Розроблено удосконалений релативістський підхід до вивчення фундаментальних параметрів спектроскопії та фотодинаміки екзотичних (піонних) атомних систем на основі рівняння Клейна-Гордона-Фока та релативістської теорії багаточастинкової збурень багатьох з урахуванням фундаментальних електромагнітних і сильних піон-ядерних взаємодій. Ефекти сильної піон-ядерної взаємодії враховуються за допомогою узагальненої моделі сильного піон-ядерного оптичного потенціалу з ефективним потенціалом Еріксона-Еріксона. Ядерний ефект скінченного розміру враховується в рамках моделі Фермі. З метою урахування впливу ядерної квадрупольної деформації на піонні динамічні процеси, використано модель Токі та ін. Радіаційні
поправки ефективно враховуються в рамках узагальненого наближення Улінга-Сербера для обробки частини поляризації вакууму Лемба. Наведені прецизійні дані для енергетичних і спектральних параметрів для піонних атомів 173Yb, 175Lu, 197Au, 208Pb, 238U з урахуванням радіаційних, ядерних (скінчений розмір ядра) поправок та ефектів сильної піон-ядерної взаємодії.

Ключові слова: релятивістська теорія, піонні атомні системи, спектроскопія та фотодинаміка

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