UDC 539.182

A. V. Glushkov

Odessa State Environmental University, L'vovskaya str.15, Odessa-16, 65016, Ukraine
E-mail: dirac13@mail.ru

RELATIVISTIC THEORY OF THE NEGATIVE MUON CAPTURE BY AN ATOM

We reviewed an effective consistent approach to determination of the cross-section for the negative muon capture by an atomic system. The approach is based on the relativistic many-body perturbation (PT) theory with using the Feynman diagram technique and a generalized relativistic energy approach in a gauge-invariant formulation. The corresponding capture cross-section is connected with an imaginary (scattering) part of the electron subsystem energy shift ImδE (till the QED perturbation theory order). The some calculation results for cross-section of the negative muon μ - capture by He atom are listed and reviewed. The theoretical and experimental studying the muon-γ-nuclear interaction effects opens prospects for nuclear quantum optics, probing the structural features of a nucleus and muon spectroscopy in atomic and molecular photophysics.

1. Introduction

Muonic atoms have always been useful tools for nuclear (atomic) spectroscopy employing atomic-physics techniques. Electrons, muons (other particles such as kaons, pions etc) originally in the ground state of the target atom can be excited reversibly either to the bound or continuum states. With appearance of the intensive neutron pencils, laser sources studying the γ-μ-nuclear interactions is of a great importance [1-20]. The rapid progress in laser technology even opens prospects for nuclear quantum optics via direct laser-nucleus coupling [19-26]. It is known that a negative muon μ^- captured by a metastable nucleus may accelerate a discharge of the latter by many orders of magnitude [18-22]. The μ-atom system differs advantageously of the usual atom; the relation r_n/r_a (r_n is a radius of a nucleus and r_a is a radius of an atom) can vary in the wide limits in dependence upon the nuclear charge. The estimates of probabilities for discharge of a nucleus with emission of γ quantum and further muon or electron conversion are presented in ref. [2-4,19,20,22]. Despite the relatively long history, studying processes of the muon-atom and muon-nucleus interactions hitherto remains very actual and complicated problem. Theoretical estimates in different models differ significantly [1-4,22]. According to Mann & Rose, the μ capture occurs mainly at the energies of E~10κeV, but according to Bayer, muons survive till thermal energies [2,20]. In many papers different authors predicted the μ capture energies in the range from a few dozens to thousands eV. The standard theoretical approach to problem bases on the known Born approximation with the plane or disturbed wave functions and the hydrogen-like functions for the discrete states. In papers by Vogel etal and Leon-Miller the well-known Fermi-Teller model is used (the atomic electrons are treated as an electron gas and a muon is classically described) [2-4]. In paper by Cherepkov and Chernysheva [2] the Hartree-Fock (HF) method is used to calculate the cross-sections of the capture, elastic and inelastic scattering of the negative μ on the He atom. In recent years more advanced approaches using the fermion molecular dynamics method are used to solve the scattering and capture problem [4,5]. The Kravtsov-Mikhailov model [4] describes transition of a muon from the excited muonic H to He based on quasimolecular concept. The series of papers by Ponomarev et al on treating the muonic nuclear catalysis use ideas of Alvarets et al [5]. More sophisticated methods of the relativistic (QED) PT should be used for correct treating the muon capture effects by multielectron atoms (nuclei). In Refs. [20] it has been presented the theoretical basis of a new relativistic energy formalism. Here we reviewed some aspects of this approach to calculation of the cross-section of the negative muon capture by atoms, using relativistic many-body PT [20,24-27] and listed some computing results for the cross-section of μ^- capture by the He atom.

2. Relativistic energy approach to the muon-atom interaction

2.1 General Formalism

In atomic theory, a convenient field procedure is known for calculating the energy shifts ΔE of the degenerate states. Secular matrix M diagonalization is used. In constructing M, the Gell-Mann and Low adiabatic formula for ΔE is used. A similar approach, using this formula with the QED scattering matrix, is applicable in the relativistic theory [20,24-27]). In contrast to the non-relativistic case, the secular matrix elements are already complex in the PT second order (first order of the inter-electron interaction). Their imaginary parts relate to radiation decay (transition) probability. The total energy shift of the state is usually presented as follows:

$$\Delta E = \mathrm{Re}\Delta E + \mathrm{i}\ \mathrm{Im}\Delta E, \tag{1a}$$

$$\mathrm{Im}\ \Delta E = -\Gamma/2, \tag{1b}$$

where Γ is interpreted as the level width, and the decay possibility $P=\Gamma$. The whole calculation of energies and decay probabilities of a non-degenerate excited state is reduced to calculation and diagonalization of the complex matrix M. To start with the Gell-Mann and Low formula it is necessary to choose the PT zero-order approximation. Usually, the one-electron Hamiltonian is used, with a central potential that can be treated as a bare potential in the formally exact QED PT. There are many well-known attempts to find the fundamental optimization principle for construction of the bare one-electron Hamiltonian (for free atom or atom in a field) or (what is the same) for the set of the one-quasiparticle (QP) functions, which represent such a Hamiltonian [24-27]. Here we consider closed electron shell atoms (ions). For example, the ground state $1s^2$ of the He atom or He-like ion. As the bare potential, one usually includes the electric nuclear potential V_N and some parameterized screening potential V_C. The parameters of the bare potential may be chosen to generate the accurate eigen-energies of all two-QP states. In the PT second order the energy shift is expressed in terms of the two-QP matrix elements [20,24-27]:

$$V(1,2;4,3) = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)}\cdot$$

$$\cdot(-1)^{j_1+j_2+j_3+j_4+m_1+m_2}\,. \tag{2}$$

$$\times\sum_{\lambda,\nu}(-1)^{\nu}\begin{bmatrix} j_1 \ldots\ldots j_3 \ldots \lambda \\ m_1 .-m_3 .. \nu\end{bmatrix}\begin{bmatrix} j_2 \ldots\ldots j_4 \ldots \lambda \\ m_2 .-m_4 .. \nu\end{bmatrix} Q_\lambda^{Qul}$$

Here Q_λ^{Qul} is corresponding to the Coulomb inter-particle interaction:

$$Q_\lambda^{Qul} = \{R_\lambda(1243)S_\lambda(1243) + R_\lambda(\tilde{1}24\tilde{3})S_\lambda(\tilde{1}24\tilde{3}) + R_\lambda(1\tilde{2}\tilde{4}3)S_\lambda(1\tilde{2}\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})\}, \tag{3}$$

where $R_\lambda(1,2;4,3)$ is the radial integral of the Coulomb inter-QP interaction with large radial Dirac components; the tilde denotes a small Dirac component; S_λ is the angular multiplier (see details in Refs.[20,24-30]). To calculate all necessary matrix elements one must have the 1QP relativistic functions. Further we briefly outline the main idea using, as an example, the negative muon capture by He atom: $((ls)^2[J_iM_i],\ \varepsilon_{in}^{\ \mu})\rightarrow(ls\varepsilon l,\varepsilon_{nl}^{\ \mu})$. Here J_i is the total angular moment of the initial target state; indices $\varepsilon_{in}^{\ \mu}$ and $\varepsilon_{fk}^{\ \mu}$ are the incident and discrete state energies, respectively to the incident and captured muons. Further it is convenient to use the second quantization representation. In particular, the initial state of the system "atom plus free muon" can be written as $a_n^{+\mu}\Phi_0$ state. The final state is that of an atom with the discrete state electron, removed electron and captured muon; in further $|I>$ represents one-particle (1QP) state, and $|F>$ represents the three-quasiparticle (3QP) state. The imaginary (scattering) part of the energy shift $Im\ \Delta E$ in the atomic PT second order (fourth order of the QED PT) is as follows [20,24,25]:

$$\mathrm{Im}\Delta E = \pi G(\varepsilon_{iv}, \varepsilon_{ie}, \varepsilon^{\mu}_{in}, \varepsilon^{\mu}_{fk}), \tag{4}$$

where indices *e,v* are corresponding to atomic electrons and *G* is a definite squired combination of the two-QP matrix elements (2). The value $\sigma = -2\, Im\Delta E$ represents the capture cross-section if the incident muon eigen-function is normalized by the unit flow condition. The different normalization conditions are used for the incident and captured state QP wave functions. The details of the whole numerical procedure of calculation of the cross-sections can be found in Refs. [20,24-27].

2.2 The Dirac-Kohn-Sham Relativistic Wave Functions

Usually, a multielectron atom is defined by a relativistic Dirac Hamiltonian(the a.u. used):

$$H = \sum_i h(r_i) + \sum_{i>j} V\left(r_i r_j\right). \tag{5}$$

Here, *h(r)* is one-particle Dirac Hamiltonian for electron in a field of the finite size nucleus and *V* is potential of the inter-electron interaction. The relativistic inter electron potential is as follows [20,24,25]:

$$V\left(r_i r_j\right) = exp\left(i\omega_{ij} r_{ij}\right) \cdot \frac{\left(1-\alpha_i \alpha_j\right)}{r_{ij}}, \tag{6}$$

where ω_{ij} is the transition frequency; α_i ,α_j are the Dirac matrices. The Dirac equation potential includes the electric potential of a nucleus and exchange-correlation potential. One of the variants is the Kohn-Sham-like (KS) exchange relativistic potential, which is obtained from a Hamiltonian having a transverse vector potential describing the photons, is as follows [31]:

$$V_X[\rho(r), r] = V_X^{KS}(r) \cdot \{\frac{3}{2} \ln \frac{[\beta + (\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}} - \frac{1}{2}\}, \tag{7}$$

where

$$\beta = [3\pi^2 \rho(r)]^{1/3} / c \tag{8}$$

The corresponding correlation functional is [20,31]:

$$V_C[\rho(r), r] = -0.0333 \cdot b \cdot \ln[1 + 18.3768 \cdot \rho(r)^{1/3}], \tag{9}$$

where *b* is the optimization parameter (see details in Refs. [20,27,32]). Earlier it has been shown [27-32] that an adequate description of the atomic characteristics requires using an optimized base of the wave functions. In Ref. [24b] a new ab initio optimization procedure is proposed. It is reduced to minimization of the gauge dependent multielectron contribution $Im\Delta E_{ninv}$ of the lowest QED PT corrections to the radiation widths of atomic levels. In the fourth order of QED PT (the second order of the atomic PT) there appear the diagrams, whose contribution to the $Im\Delta E_{ninv}$ accounts for correlation effects. This contribution is determined by the electromagnetic potential gauge (the gauge dependent contribution). All the gauge dependent terms are multielectron by their nature. The dependent contribution to imaginary part of the electron energy is obtained after involved calculation, as [24b]:

$$\begin{aligned} Im\delta E_{ninv}(\alpha - s|b) = {} & -C\frac{e^2}{4\pi}\iiiint dr_1 dr_2 dr_3 dr_4 \sum_{n>f, m\le f} \left(\frac{1}{\omega_{mn}+\omega_{\alpha s}} + \frac{1}{\omega_{mn}-\omega_{\alpha s}}\right) \\ & \times \Psi^+_\alpha(r_1)\Psi^+_m(r_2)\Psi^+_s(r_4)\Psi^+_n(r_3) \cdot [(1-\alpha_1\alpha_2)/r_{12}] \cdot \{[\alpha_3\alpha_4 - (\alpha_3 n_{34})(\alpha_4 n_{34})]/r_{34} \\ & \times \sin[\omega_{\alpha n}(r_{12}+r_{34})] + [1 + (\alpha_3 n_{34})(\alpha_4 n_{34})]\omega_{\alpha n} \cos[\omega_{\alpha n}(r_{12}+r_{34})]\} \\ & \times \Psi_m(r_3)\Psi_\alpha(r_4)\Psi_n(r_2)\Psi_s(r_1). \end{aligned} \tag{10}$$

Here, *C* is the gauge constant, *f* is the boundary of the closed shells; $n \ge f$ indicating the vacant band and the upper continuum electron states; $m \le f$ indicates the finite number of states in the atomic core). The minimization of the $Im\Delta E_{ninv}$ leads to the Dirac-like equations. In concrete calculation it is sufficient to use the simplified procedure, which is reduced to the functional minimization using the variation of the parameter *b* in Eq.(9) [20,25].

2.3 Capture of negative muons by helium atom

The results of calculation of the cross-section for the negative muon capture by atom of He are shown in Figures 1-3. The scheme includes 2×10^3 points till distance $25a_B$ (a_B is the Bohr radius). The main contribution to the capture cross-section is provided by transitions with the moment *l*=0-3.

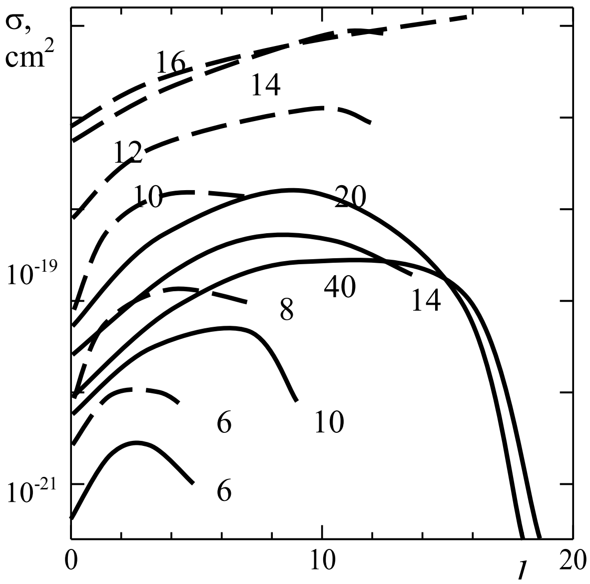

Figure 1. The calculated dependences of the Auger capture cross-section (solid line– E=50eV; dotted line - E=20eV) on orbital number *l* for different *n* values for incident μ^- energies 20, 50 eV (from Refs. [2-4,20]).

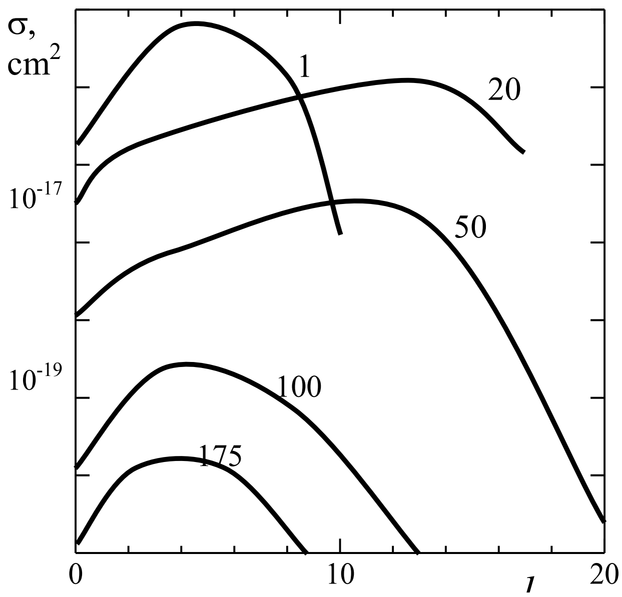

Figure 2. The capture cross-sections in dependence on the orbital number l after summation on the n number (digits in figure – the muon energies in eV; from Refs. [2-4,20]).

First we studied the behaviour of curves of the μ^- capture cross-section in dependence on the principal quantum number *n* with summation on the orbital moments *l* for several values of the muon initial energy. In whole our curves are lying a little higher than the corresponding curves of Refs. [1-3]. The analysis shows that for the incident μ energies 16 and 50eV the capture cross-section begins to decrease for all *n* with growth of the *l* number (l>10). The states with large *l* for the muon energies (lower or higher in comparison with the atomic ionization potential value) are populated less probably than in a case of the μ^- energy of the ionization potential order. In figure 1we present the calculated dependences of the Auger capture cross-section on the orbital number *l* for different *n* values for the incident μ energies of 20 and 50 eV. In figure 2 we present the calculated capture cross-section in the dependence on the *l* number after summation on *n*.

In figure 3 we present the total capture cross-section in terms of energy (with summation on all *n,l*): data on the Auger capture cross-section – curve 7 (elastic and inelastic scattering cross-sections) – curves 2,3 [20]. We also present the results by Copenman and Rogova in the Born approximation with using the hydrogen-like wave functions (curve 5) and the HF data [2] (curve 1), the inelastic scattering cross-section by Rosenberg (curve 4), the transport cross-section (x symbol) [2,3,20]. The analysis of the results shows that the data [2-4, 20] are in physically reasonable agreement. But, there is an essential difference of the Mann-Rose and Bayer data [1-3].

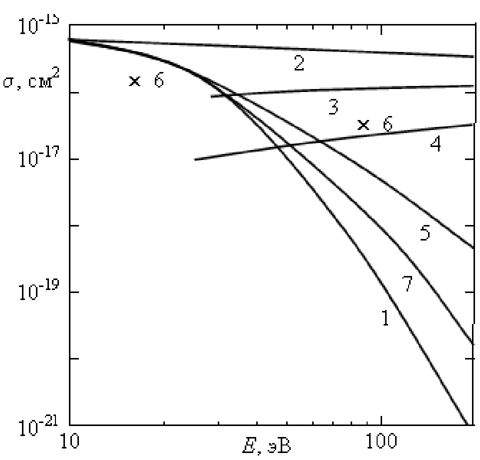

Figure 3. Total cross-section of μ^- capture in dependence on an energy: the Auger capture cross-section – curve 7; elastic and inelastic scattering cross-sections – curves 2,3 by Glushkov et al; cross-section of capture by Copenman and Rogova (curve 5); the HaF data by Cherepkov-Chernysheva – curve 1; inelastic scattering cross-section by Rosenberg – curve 4; the transport cross-section – x (from Refs. [2-4,20]).

The relativistic corrections were to found to be small here, but computing heavy atoms (nuclei) requires a proper treatment for both relativistic and correlation effects.

3 Concluding Remarks and Future Perspectives

We have presented a new relativistic approach to calculation of the cross-section of the negative μ capture by atoms. The approaches are based upon the relativistic many-body PT theory, energy approach. Note that further development of electron-μ-nuclear spectroscopy of atoms (nuclei) is of a great theoretical and practical interest. The development of new approaches [2-6,21-23] to studying the cooperative e-,μ-γ-nuclear processes promises the rapid progress in our understanding of the nuclear decay. Such an approach is useful, providing perspective for search for new cooperative effects on the boundary of atomic and nuclear physics, carrying out new methods for treating (the muonic chemistry tools) the spatial structure of molecular orbitals, studying the chemical bond nature and checking different models in quantum chemistry and atomic physics [3-8,18-23,49].

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This article has been received in April 2016.

UDC 539.182

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RELATIVISTIC ENERGY APPROACH TO THE NEGATIVE MUON CAPTURE BY AN ATOM

Abstract

We reviewed a new effective consistent approach to determination of the cross-section for the negative muon capture by an atomic system. The approach is based on the relativistic many-body perturbation (PT) theory with using the Feynman diagram technique and a generalized relativistic energy approach in a gauge-invariant formulation. The corresponding capture cross-section is connected with an imaginary (scattering) part of the electron subsystem energy shift ImδE (till the QED perturbation theory order). The some calculation results for cross-section of the negative muon μ^- capture by He atom are listed and reviewed. The theoretical and experimental studying the muon-γ-nuclear interaction effects opens prospects for nuclear quantum optics, probing the structural features of a nucleus and muon spectroscopy in atomic and molecular photophysics.

Key words: Cooperative muon-γ-nuclear processes, muon capture by an atom, Relativistic energy formalism

УДК 539.182

А. В. Глушков

РЕЛЯТИВИСТСКИЙ ЭНЕРГЕТИЧЕСКИЙ ПОДХОД К ОПИСАНИЮ ПРОЦЕССА ЗАХВАТА ОТРИЦАТЕЛЬНОГО МЮОНА АТОМОМ

Резюме

В работе обзорно изложены основы нового эффективного подхода к определению сечений захвата отрицательного мюона атомной системой, основанного на релятивистской многочастичной теории возмущения с использованием фейнмановской диаграммной техники и обобщенном релятивистском энергетическом формализме в калибровочно-инвариантной формулировке. Соответствующее сечение захвата отрицательного мюона атомом определяется мнимой частью энергетического сдвига ImδE электронной подсистемы. Обзорно представлены результаты некоторых расчетов сечения захвата отрицательного мюона атомом He. Теоретическое и экспериментальное изучение эффектов мюон-гамма-ядерных взаимодействий открывает перспективы развития новой области квантовой оптики, а именно, ядерной квантовой оптики, возможности зондирования структурных особенностей ядра (атома) и дальнейшего развития направления мюонной спектроскопии в атомной и молекулярной физике.

Ключевые слова: кооперативные мюон-гамма-ядерные процессы, захват мюона атомом, релятивистский энергетический формализм

УДК 539.182

О. В. Глушков

РЕЛЯТИВІСТСЬКИЙ ЕНЕРГЕТИЧНИЙ ПІДХІД ДО ОПИСУ ПРОЦЕСА ЗАХОПЛЕННЯ НЕГАТИВНОГО МЮОНА АТОМОМ

Резюме

У роботі оглядово викладені основи нового ефективного підходу до визначення перетинів захоплення негативного мюона атомної системою, заснованого на релятивістській багаточастинковій теорії збурень з використанням фейнманівськох діаграмної техніки і узагальненому релятивістському енергетичному формалізмі у калібрувально-інваріантному формулюванні. Відповідний перетин захоплення негативного мюона атомом визначається уявною частиною енергетичного зсуву ImδE електронної підсистеми. Оглядово представлені результати деяких розрахунків перетину захоплення негативного мюона атомом гелія. Теоретичне і експериментальне вивчення ефектів мюон-гамма-ядерних взаємодій відкриває перспективи розвитку нової галузі квантової оптики, а саме, ядерної квантової оптики, нові можливості зондування структурних особливостей ядра (атома) і подальшого розвитку напрямку мюонної спектроскопії в атомній і молекулярної фотофізиці.

Ключові слова: кооперативні мюон-гамма-ядерні процеси, захоплення мюона атомом, релятивістський енергетичний формалізм