МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Quantum Optics and Laser Physics", Part 4. (Training of PhD students of the specialty: 104 –"Physics and astronomy")

«Затверджено»
на засіданні групи забезпечення спеціальності
Протокол №1 від 28/08/2021 Голова групи _____ Свинаренко А.А.

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

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Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline “Quantum Optics and Laser Physics”, Part 2. (Training of PhD students of the specialty: 104 –“Physics and astronomy”)

Compilers:
Glushkov O.V., D.f.-m.s.(Hab.Dr.), prof., Head of the department of higher and applied mathematics (OSENU)
Khetselius O.Y., d.f.-m.s.(HabD), prof., Prof. of the department of higher and applied mathematics (OSENU)
Svinarenko A.A., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Editor:
Svinarenko A.A., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU), Guarantor of educational and scientific training program for the PhD Students on specialty 104 - “Physics and Astronomy”; 01.04.05- “Optics and Laser Physics”

PREFACE

The discipline "Quantum Optics and Laser Physics" is a mandatory discipline in the cycle of professional training of graduate students (third level of education) in the specialty 104-Physics and Astronomy.

It is aimed at mastering (providing) a number of planned competencies, including the study of modern quantum optics and laser physics, as well as new methods of describing, modeling, predicting the properties of light radiation, its propagation, absorption, refraction and reflection in different environments. nature, research of atomic and molecular spectra, interaction of electromagnetic radiation with atoms, molecules, solids, formation of coherent light sources, optical recording of information, etc. and achievement of scientific results that create potentially new knowledge.

The place of the discipline in the structural and logical scheme of its teaching: the knowledge gained in the study of this discipline is used in the study of another compulsory discipline "Computational methods of optics and dynamics of quantum and laser systems" and elective disciplines "Atomic optics and spectroscopy", "Molecular optics" and spectroscopy "," Optics and spectroscopy of a solid body "in the cycle of professional training of graduate students. The basic concepts of the discipline are the obligatory tools of an experienced specialist in the field of physics and astronomy, in particular, optics and laser physics.

The purpose of the discipline is to master (provide) a number of competencies, in particular, mastering the modern apparatus of optics and laser physics, the ability to develop and use new approaches in the theory of light radiation, its propagation, absorption, in environments, research of atomic and molecular spectra, electromagnetic interaction radiation with atoms, molecules, solids, the formation of coherent light sources, optical recording of information, The total amount of study time for the study of the discipline is 300 hours. for full-time education and 300 hours. for distance learning.

After mastering this discipline, the graduate student must be able to develop and use new approaches in the theory of light radiation, its propagation, absorption, in environments of different nature, study of atomic and molecular spectra, interaction of electromagnetic radiation with atoms, molecules, solids, use modern scientific methods results that create new knowledge.

The main topics are as follows: Solid state and atomic spectroscopy. Transitions in the electronic subsystem. Auger and Fano effects

Topics: Solid state and atomic spectroscopy. Transitions in the electronic subsystem Auger and Fano effects

Топіки: Спектроскопія твердого тіла. Переходи в електронній підсистемі Ефекти Оже і Фано **(ЗБ- Л8)**

I.1 Introduction

The Auger electron spectroscopy is an effective method to study the chemical composition of solid surfaces and near-surface layers etc [1-8]. Sensing the Auger spectra in atomic systems and solids gives the important data for the whole number of scientific and technological applications. When considering the method principles, the main attention is given as a rule to the models for drawing chemical information from the Auger spectra and to the surface composition determination methods by the Auger spectrum decoding. It is just the two-step model that is used most widely when calculating the Auger decay characteristics. Since the vacancy lifetime in an inner atomic shell is rather long (about 10^{-17} to 10^{-14}s), the atom ionization and the Auger emission are considered to be two independent processes. In the more correct dynamic theory of the Auger effect [1-4] the processes are not believed to be independent from one another. The fact is taken into account that the relaxation processes due to Coulomb interaction between electrons and resulting in the electron distribution in the vacancy field have no time to be over prior to the transition. In fact, a consistent Auger decay theory has to take into account correctly a number of correlation effects, including the energy dependence of the vacancy mass operator, the continuum pressure, spreading of the initial state over a set of configurations etc. [9-20]. Note that the effects are not described adequately to date, in particular within the Auger decay theory [2].

The most widespread theoretical studying the Auger spectra parameters is based on using the multi-configuration Dirac-Fock (MCDF) calculation [1-3]. The theoretical predictions based on MCDF calculations have been carried out within different approximations and remained hitherto non-satisfactory in many relations. Earlier [11,12] it has been proposed relativistic perturbation theory (PT) method of the Auger decay characteristics for complex atoms, which is

based on the Gell-Mann and Low S-matrix formalism energy approach and many-body perturbation theory (PT) formalism [4-7]. The novel element was in using the optimal basis of the electron state functions derived from the minimization condition for the calibration-non-invariant contribution (the second order PT polarization diagrams contribution) to the imaginary part of the multi-electron system energy already at the first non-disappearing approximation of the PT. Earlier it has been applied in studying the Auger decay characteristics for a set of neutral atoms and quasi-molecules. Besides, the ionization cross-sections of inner shells in various atoms and the Auger electron energies in solids were estimated. In this paper the combined relativistic energy approach and relativistic many-body PT with the zeroth order density functional approximation is used for sensing the Auger spectra of solids and calculation of their energy parameters..

I.2 The theoretical method

In Refs. [4,5,16-22] the fundamentals of the relativistic many-body PT formalism have been in detail presented, so further we are limited only by the novel elements. Let us remind that the majority of complex atomic systems possess a dense energy spectrum of interacting states. In Refs. [1,3-5] there is realized a field procedure for calculating the energy shifts ΔE of degenerate states, which is connected with the secular matrix M diagonalization. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the complex secular matrix. In the relativistic energy approach [4-9], which has received a great applications during solving numerous problems of atomic, molecular and nuclear physics (e.g., see Refs. [1,4,5,23-30]), the imaginary part of electron energy shift of an atom is directly connected with the radiation decay possibility (transition probability).

An approach, using the Gell-Mann and Low formula with the QED scattering matrix, is used in treating the relativistic atom. The total energy shift of the state is usually presented in the form:

$$\Delta E = \mathrm{Re}\Delta E + i\,\Gamma/2\,, \qquad (1)$$

where Γ is interpreted as the level width, and the decay possibility P = Γ. The imaginary part of electron energy of the system, which is defined in the lowest order of perturbation theory as [4]:

$$\mathrm{Im}\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V_{\alpha n \alpha n}^{|\omega_{\alpha n}|}, \qquad (2)$$

where (α>n>f) for electron and (α<n<f) for vacancy; $V_{\alpha n \alpha n}^{|\omega|}$ is an imaginary part of the matrix element of the potential:

$$V(r_i r_j) = exp(i\omega r_{ij}) \cdot \frac{(1-\alpha_i \alpha_j)}{r_{ij}} \qquad (3)$$

Within the frame of the relativistic PT approach the Auger transition probability and the Auger line intensity are defined by the square of an electron interaction matrix element having the form [2-4]:

$$V_{1234}^{\omega} = [(j_1)(j_2)(j_3)(j_4)]^{1/2} \sum_{\lambda\mu} (-1)^{\mu} \begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times \mathrm{Re} Q_{\lambda}(1234);$$

$$Q_{\lambda} = Q_{\lambda}^{\mathrm{Qul}} + Q_{\lambda}^{\mathrm{Br}}. \qquad (5)$$

The terms $Q_{\lambda}^{\mathrm{Qul}}$ and $Q_{\lambda}^{\mathrm{Br}}$ correspond to subdivision of the potential into Coulomb part $cos|\omega|r_{12}/r_{12}$ and Breat one, $cos|\omega|r_{12}\alpha_1\alpha_2/r_{12}$. The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions:

$$\frac{\cos|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0} (\lambda) J_{\lambda+1/2}(|\omega| r_<) J_{-\lambda-1/2}(|\omega| r_>) P_{\lambda}(\cos \mathbf{r}_1 \mathbf{r}_2) \qquad (6)$$

where J is the 1st order Bessel function, (λ)=2λ+1.

The Coulomb part Q_λ^{Qul} is expressed in terms of radial integrals R_λ, angular coefficients S_λ according to Refs. [4]. The Breat interaction is known to change considerably the Auger decay dynamics in some cases. The Breat part of Q is defined in [2-4].

The Auger width is obtained from the adiabatic Gell-Mann and Low formula for the energy shift [3]. The direct contribution to the Auger level width with a vacancy $n_\alpha l_\alpha j_\alpha m_\alpha$ is as follows:

$$\sum_\lambda \frac{2}{(\lambda)(j_\alpha)} \sum_{\beta\gamma\le f} \sum_{k>f} Q_\lambda(\alpha k\gamma\beta) Q_\lambda(\beta\gamma k\alpha), \tag{7}$$

while the exchange diagram contribution is:

$$\frac{2}{(j_\alpha)} \sum_{\lambda_1\lambda_2} \sum_{\beta\gamma\le f} \sum_{k>f} Q_{\lambda_1}(\alpha k\gamma\beta) Q_{\lambda_2}(\beta\gamma k\alpha) \begin{Bmatrix} j_\alpha & j_\gamma & \lambda_2 \\ j_k & j_\beta & \lambda_1 \end{Bmatrix} \tag{8}$$

The partial items of the $\sum_{\beta\gamma} \sum_k$ sum answer to contributions of $\alpha^{-1} \to (\beta\gamma)^{-1} K$ channels resulting in formation of two new vacancies $\beta\gamma$ and one free electron k: $\omega_k = \omega_\alpha + \omega_\beta - \omega_\alpha$. The calculating of all matrix elements, wave functions, Bessel functions etc is reduced to solving the system of differential equations. The formulas for the autoionization (Auger) decay probability include the radial integrals $R_\alpha(\alpha k\gamma\beta)$, where one of the functions describes electron in the continuum state. When calculating this integral, the correct normalization of the wave functions is very important, namely, they should have the following asymptotic at $r \to 0$:

$$\begin{Bmatrix} f \\ g \end{Bmatrix} \to (\lambda\omega)^{-1/2} \begin{cases} \left[\omega + (\alpha Z)^{-2}\right]^{-1/2} \sin(kr + \delta), \\ \left[\omega - (\alpha Z)^{-2}\right]^{-1/2} \cos(kr + \delta). \end{cases} \tag{9}$$

The important aspect of the whole procedure is an accurate accounting for the exchange-correlation effects. We have used the generalized relativistic Kohn-

Sham density functional [3-5] in the zeroth approximation of relativistic PT; naturally, the perturbation operator contents the operator (7) minus the cited Kohn-Sham density functional. Further the wave functions are corrected by accounting of the first order PT contribution. Besides, we realize the procedure of optimization of relativistic orbitals base. The main idea is based on using ab initio optimization procedure, which 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.

The energy of an electron formed due to a transition *jkl* is defined by the difference between energies of atom with a hole at *j* level and double-ionized atom at *kl* levels in final state:

$$E_A(jkl,^{2S+1}L_J) = E_A^+(j) - E_A^{2+}(kl,^{2S+1}L_J) \tag{10}$$

In the solids theory, to single out the important correlation and medium effects, the equation (10) is usually rewritten as:

$$E_A(jkl,^{2S+1}L_J) = E(j) - E(k) - E(l) - \Delta(k,l;^{2S+1}L_J), \tag{11}$$

where the item Δ takes into account the dynamic correlation effects (relaxation due to hole screening with electrons etc.) To take these effects into account, the set of procedures elaborated in the atomic theory [3-5,11,12] is used. All calculations are performed on the basis of the modified numeral code Superatom (version 93).

I.3. Results and conclusions

Below we present the advanced data for Auger electron energy in some solids. As mentioned above, the exit probability of Auger electrons from an atom via different channels associated with ionization from a core level is defined by the matrix element (1). In addition, the proportionality coefficient in the equation coincides with the electron impact ionization cross-section σ_j of the level *j*. Of course, two aspects are to be considered when determining the exit probability of Auger electrons from an atom, namely, the radiative transition

under neutralization of a hole at the level *j* and the possibility of a considerable change in the initial hole distribution at the core levels at the Auger decay via the radiative channel jkl associated as a rule with a considerable distinctions in the non-radiative transition probabilities [11,12]. For definiteness sake, let the ionization of L levels in a multi-electron atom be considered. The probability of the Auger electron emission from the atom via the channel L_3Kl (taken as an example) is defined by the ionization cross-section of the level L_3 as well as by a certain effective cross-section depending on the ionization cross-sections of the levels L_1,L_2.

The Auger line intensity is defined by three atomic constants: $A_{jkl}=\sigma_j f_j a_{jkl}$, where a_{jkl} is the non-radiative transition probability; *fi* is the Korster-Kronig coefficient; σ_j , the ionization cross-section defined by the matrix element (1) calculated for wave functions of bound state and continuum one. In table 1 we present the data on Auger electron energy for some solids calculated using the presented approach (column C), the semi-empirical method with using the Larkins' equivalent core approximation [8] (column A), the perturbation theory approach [11,12] as well as experimental data (c.g.[1]).

Table 1.

Experimental data for Auger electron energy for solids and calculated values (A, semi-empirical method [1]; B, [11,12]; C- present)

Ele-ment	Auger line	Experiment	Theory: A	Theory: B	Theory : C
Na	$KL_{2,3}L_{2,3}\ ^1D_2$	994.2	993.3	994.7	994.1
Si	$KL_{2,3}L_{2,3}\ ^1D_2$	1616.4	1614.0	1615.	1616.2
Ge	$L_3M_{4,5}M_{4,5}$	1146.2	1147.2	9	1146.1
Ag	$^1G_4$	353.4	358.8	1146.	353.2
	$M_5N_{4,5}N_{4,5}$			6	
	$^1G_4$			354.1	

The calculation accuracy using method [1] is within about 2 eV as an average. Our approach provides more accurate results that is provided by more correct accounting for complex electron interaction. Some improvement of the

present data in comparison with results [9,10] is connected using the optimized one-quasiparticle representation in the relativistic many-body perturbation theory, which significantly affects an agreement between theory and experiment.

. To conclude, let us note [12] that using the Auger electron spectroscopy in analysis of the surface chemical composition and elements [1,3,30-34] requires consideration of Auger spectra and the corresponding characteristics of the Auger transitions, interpretation of effects like the shape transformations of the valence Auger spectra due to appearance of new lines, position and intensity changes of individual lines caused by the redistribution in the electron state density of the valence band. The correct theoretical estimations of the spectral characteristics are of critical importance for their full understanding.

2. Tests performance

Test Option 1.

1). Give the key definitions of the solid state and atomic Auger spectroscopy, and the Auger and Fano effects; Describe the fundamental topics of the relativistic energy approach (S-matrix adiabatic Gell-Mann and Low formalism) to autoionization and Auger spectroscopy for atoms and solids.

2) Explain the main points of the Auger spectroscopy of atomic system and solids: i) mathematical and physical essense of Auger effect; ii) calculation of the Auger transitions energies; iii) calculation of the Auger widths within relativistic energy approach; iv) the key features of the computational realization of the approach.

3). Construct the consistent theoretical model for calculating the Auger transitions energies and Auger widths (on example of **sodium)**.

4). Perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom”) your theoretical model for calculating the Auger transitions energies and Auger widths parameters (on example of **sodium)**.

Test Option 2.

1). Give the key definitions of the solid state and atomic Auger spectroscopy, and the Auger and Fano effects; Describe the fundamental topics of the relativistic energy approach (S-matrix adiabatic Gell-Mann and Low formalism) to autoionization and Auger spectroscopy for atoms and solids.

2) Explain the main points of the Auger spectroscopy of atomic system and solids: i) mathematical and physical essense of Auger effect; ii) calculation of the Auger transitions energies; iii) calculation of the Auger widths within relativistic energy approach; iv) the key features of the computational realization of the approach.

3). Construct the consistent theoretical model for calculating the Auger transitions energies and Auger widths (on example of **magnesium)**.

3). Perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom”) your theoretical model for calculating the Auger transitions energies and Auger widths parameters (on example of **magnesium)**.

Test Option 3.

1). Give the key definitions of the solid state and atomic Auger spectroscopy, and the Auger and Fano effects; Describe the fundamental topics of the relativistic energy approach (S-matrix adiabatic Gell-Mann and Low formalism) to autoionization and Auger spectroscopy for atoms and solids.

2) Explain the main points of the Auger spectroscopy of atomic system and solids: i) mathematical and physical essense of Auger effect; ii) calculation of the Auger transitions energies; iii) calculation of the Auger widths within relativistic energy approach; iv) the key features of the computational realization of the approach.

3). Construct the consistent theoretical model for calculating the Auger transitions energies and Auger widths (on example of **calcium)**.

4). Perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom”) your theoretical model for calculating the Auger transitions energies and Auger widths parameters (on example of **calcium)**.

Test Option 4.

1). Give the key definitions of the solid state and atomic Auger spectroscopy, and the Auger and Fano effects; Describe the fundamental topics of the relativistic energy approach (S-matrix adiabatic Gell-Mann and Low formalism) to autionizayion and Auger spectroscopy for atoms and solids.

2) Explain the main points of the Auger spectroscopy of atomic system and solids: i) mathematical and physical essense of Auger effect; ii) calculation of the Auger transitions energies; iii) calculation of the Auger widths within relativistic energy approach; iv) the key features of the computational realization of the approach.

3). Construct the consistent theoretical model for calculating the Auger transitions energies and Auger widths (on example of **rubidium)**.

3). Perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom”) your theoretical model for calculating the Auger transitions energies and Auger widths parameters (on example of **rubidium)**.

Test Option 5.

1). Give the key definitions of the solid state and atomic Auger spectroscopy, and the Auger and Fano effects; Describe the fundamental topics of the relativistic energy approach (S-matrix adiabatic Gell-Mann and Low formalism) to autoionization and Auger spectroscopy for atoms and solids.

2) Explain the main points of the Auger spectroscopy of atomic system and solids: i) mathematical and physical essense of Auger effect; ii) calculation of the Auger transitions energies; iii) calculation of the Auger widths within relativistic energy approach; iv) the key features of the computational realization of the approach.

3). Construct the consistent theoretical model for calculating the Auger transitions energies and Auger widths (on example of **stronium)**.

4). Perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom”) your theoretical model for calculating the Auger transitions energies and Auger widths parameters (on example of **stronium)**.

Test Option 6.

1). Give the key definitions of the solid state and atomic Auger spectroscopy, and the Auger and Fano effects; Describe the fundamental topics of the relativistic energy approach (S-matrix adiabatic Gell-Mann and Low formalism) to autoionization and Auger spectroscopy for atoms and solids.

2) Explain the main points of the Auger spectroscopy of atomic system and solids: i) mathematical and physical essense of Auger effect; ii) calculation of the Auger transitions energies; iii) calculation of the Auger widths within relativistic energy approach; iv) the key features of the computational realization of the approach.

3). Construct the consistent theoretical model for calculating the Auger transitions energies and Auger widths (on example of **francium)**.

3). Perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom”) your theoretical model for calculating the Auger transitions energies and Auger widths parameters (on example of **francium)**.

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Compiler:
Glushkov O.V., D.f.-m.s.(Hab.Dr.), prof., Head of the department of higher and applied mathematics (OSENU)
Khetselius O.Y., d.f.-m.s.(HabD), prof., Prof. of the department of higher and applied mathematics (OSENU)
Svinarenko A.A., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Editor:
Svinarenko A.A., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU), Guarantor of educational and scientific training program for the PhD Students on specialty 104 - "Physics and Astronomy"; 01.04.05- "Optics and Laser Physics"

Odessa State Environmental University
65016, Odessa, L'vovskaya str., 15, Room 406 (1st bld.)