МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

**Methodical instructions
for practical work, test performance, distance
learning of PhD students in the discipline "Molecular Optics
and Spectroscopy", Part 7 (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
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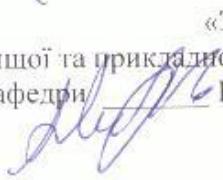
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THE MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE
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Methodical instructions
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Odessa 2021

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Molecular Optics and Spectroscopy", Part 7. (Training specialty: 104 - "Physics and Astronomy"; 01.04.05- "Optics and Laser Physics" and others)

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PREFACE

Discipline "Molecular optics and spectroscopy" is a compulsory discipline in the cycle of professional training of postgraduate students (3 level of education) in specialty 104 – Physics and Astronomy (specialization: 01.04.05 -optics and laser physics). **It is aimed at** assimilating (assuring) a number of planned competences, including the study of the modern apparatus of molecular optics and spectroscopy, as well as the development of new computational methods of determination and treating spectra of diatomic and multiatomic molecules, their energetic and spectroscopic characteristics on the basis of methods of quantum mechanics and quantum electrodynamics, the ability to analyze data of numerical experiments on the study of molecular energetic, optical, spectroscopic characteristics that can be large and require the use of powerful computing resources, the use of modern existing and new advanced methods in order to achieve scientific results that create potentially new knowledge in Molecular optics and spectroscopy.

The place of discipline in the structural-logical scheme of its teaching: the knowledge gained during the study of this discipline is used in the writing of dissertations, the topics of which are related to determination and treating spectra of diatomic and multiatomic molecules, their energetic and spectroscopic characteristics on the basis of methods of quantum mechanics and quantum electrodynamics. **The basic concepts** of discipline are the fundamental tools of a specialist in the field of Physics and Astronomy (specialization: 01.04.05 - optics and laser physics).

The purpose of studying the discipline is assimilation (assurance) of a number of competencies, in particular, the achievement of the relevant knowledge, understanding and the ability to use the advanced methods of molecular optics and spectroscopy, as well as the development of new computational methods of determination and treating spectra of diatomic and multiatomic molecules, their energetic and spectroscopic characteristics on the basis of methods of quantum mechanics and quantum electrodynamics, to the needs of the dissertation before - study, adapt, improve quantum (molecular) methods to analyze data on molecular spectra, results of numerical experiments on the study of molecular energetic, optical, spectroscopic characteristics.

After mastering this discipline, the postgraduate student must be able to use modern or personally developed new methods, in particular, to analyze, simulate, predict, and program the spectra of diatomic and multiatomic molecules. These methodical instructions are for the second-year PhD students and tests performance in the discipline «Molecular optics and spectroscopy».

The main topics: Relative population of Vibrational energy levels. Relative population of rotational energy levels. Vibrational structure of electronic bands. Intensity distribution in cooperative electron-vibrational spectra.

Topics: Relative population of Vibrational energy levels. Relative population of rotational energy levels. Vibrational structure of electronic bands. Intensity distribution in cooperative electron-vibrational spectra.

Топіки: Відносна заселеність коливальних рівнів енергії. Відносна заселеність обертальних рівнів енергії. Коливальна структура електронних смуг. Електронні переходи двоатомних молекул. Коливальна структура електронних смуг. Розподіл інтенсивності в електронно-коливальних спектрах. (ЗБ- Л1.6)

1. Elements of theory of cooperative electron-vibrational spectra

The different aspects of the molecular spectroscopy are in details presented in Refs. [1-64]. The fundamental provisions of a quantum radiation theory, in particular, the use of the Fermi golden rule and simple models such as harmonic oscillators to describe the potential curves of molecules and to determine the corresponding wave functions of vibrational-rotational states are significantly generalized.

The standard Letokhov-Minogin model assumptions provide the following points [30,31]. For certainty, it is assumed that γ-quantum interacts with the nucleus 1 of diatomic molecule consisting of nuclei 1 and 2, and let's denote the r_n as coordinates of nucleons of the nucleus 1 in the system of the center of mass (CM) of molecules, r_n' - coordinates of nucleons in CM system of nucleus 1, r_e - coordinates of electrons in CM system of molecules and through R_1 and R_2 - coordinates of CM of nucleons 1 and 2 relatively to CM of molecule.

Then, as usual, let $\Psi(r_n)$ - wave function of the nucleon system of the nucleus 1. In the adiabatic approximation, it is natural to write the wave function of a diatomic molecule in the form: $\Psi(r_e)\,\Psi(R_1, R_2)$, where $\Psi(r_e)$ - wave function of electrons, $\Psi(R_1, R_2)$ - wave function of nucleus.

The latter is determined in the Letokhov-Minogin model [30] in a harmonious approximation. Looking ahead, note that our model differs significantly from the Letokhov-Minogin model in determining the wave functions of nuclei (electrons), since the corresponding wave functions in our models are found as solutions of the Schrödinger radial equation with a realistic interatomic potential of a diatomic molecule, which is described, for example, in the density

functional approximation or the model potential one, such as the Simons-Parr-Finlan approximation [37-41].

This is the main fundamental difference between the cited approaches.

Probability of γ-transition "*a*"→"*b*" with a change in the quantum state of the optical electron "*i*"→"*f*" in the atom (molecule) is given in general terms:

$$W_{fi}^{ba} = A_{ba} \left| \langle \Psi_f^*(\vec{r}) \left| e^{-i\vec{k}_\gamma \vec{R}} \right| \Psi_i(\vec{r}) \rangle \right|^2 = A_{ba} P_{fi}, \qquad (1)$$

where A_{ba} - probability of γ-transition "*a*"→"*b*" between two levels of a free nucleus, $\vec{k}_\gamma$- wave vector of γ-quantum, $\psi_i(\vec{r})$ - wave functions describing the state of the electron, and coordinates $\vec{r}$ and $\vec{R}$ are related by the ratio of

$$\vec{R} + \frac{m}{M}\vec{r} = 0$$

type, where $\vec{r}$- the coordinate of the electron, $\vec{R}$- the coordinate of the nucleus center of the mass.

With some simplifications, the expression for the probability of a cooperative electron – gamma - nuclear transition can be reduced to the following standard form:

$$P_{fi} = (k_\gamma \frac{m}{M})^2 \left| \langle \Psi_f^*(\vec{r}) | \vec{n}_\gamma \vec{r} | \Psi_i^*(\vec{r}) \rangle \right|^2 = (k_\gamma \frac{m}{M})^2 (\vec{r}_{if} \vec{n}_\gamma)^2 \qquad (2)$$

where $i{\neq}f$, $\vec{n}_\gamma$ - single vector in the direction $\vec{k}_\gamma$, $\vec{r}_{if}$ - matrix element of the dipole moment of transition "*i*"→"*f*".

The probability of preserving the initial state of the atom $P_{fi}{<<}1$. A simple correlation that links the intensity of the satellite and the main transition line can be estimated on the basis of the simple formula by Ivanov-Letohov-Ivanov [7,8,29-31]:

$$K_{on} = \varepsilon_{on}[eV] (f_{on} E_\gamma [MeV]/A)^2, \qquad (3)$$

where ε_{on} - energy of electronic transition "*0*"→"*n*" in eV, f_{on} – oscillator strength of transition "*0*"→"*n*", A - atomic mass in atomic units.

Hamiltonian of γ-radiation interaction with a nucleon system of the nucleus 1 can usually be expressed in nucleon coordinates r'_n in CM system of nucleus 1:

$$H(r_n) = H(r'_n) exp\,(-i k_\gamma R_1),\qquad(4)$$

where k_γ - wave vector of γ-quantum.

Next, according to the standard quantum-mechanical representation, the matrix element of the transition from the initial state *"a"* in the end state *"b"* can be represented in the first order quantum mechanical PT in the form of a product of two matrix elements, one of which corresponds to a change of the internal state of the nucleus, and the other - changing the internal state of the molecule:

$$\langle \Psi_b^*(r'_n)|H(r'_n)|\Psi_a(r'_n)\rangle \cdot \langle \Psi_b^*(r_e)\Psi_b^*(R_1,R_2)\left|e^{-i\vec{k}_\gamma R_1}\right|\Psi_a(r_e)\Psi(R_1,R_2)\rangle.$$

$$(5)$$

Here the first multiplier is determined γ-the transition of the nucleus, and the second – by the matrix element of the transition of the molecule from the initial state *a* to the end state *b*:

$$M_{ba} = \langle \Psi_b^*(r_e)|\Psi_a(r_e)\rangle \cdot \langle \Psi_b^*(R_1,R_2)\left|e^{-i\vec{k}_\gamma R_1}\right|\Psi_a(R_1,R_2)\rangle\qquad(6)$$

Expression (4) is a common quantum-mechanical definition of a matrix element to calculate the probabilities of changes in the internal state of a moleculewhen radiating or absorbing γ-quantum nucleus of a molecule and determines the intensities of the corresponding γ-satellites.

Using the laws of conservation of energy and momentum, you can give energy estimates of energy E_γ of radiating or absorbing γ – quantum in diatomic molecule (see [30,37]):

$$\pm E_\gamma + E_a + \frac{1}{2Mv_n^2} = \pm E_\gamma^{(0)} + E_b + \frac{1}{2Mv^2}\qquad,\qquad(7)$$

$$Mv_0 \pm \hbar k_\gamma = Mv,\qquad(8)$$

where M – mass of molecule, v_0 and v - speed of molecule before and after the interaction of the nucleus with γ – quantum, k_γ - wave vector of γ – quantum, E_a and E_b - the internal energy of the molecule before and after the interaction, $E_\gamma^{(0)}$ -

nuclear transition energy; the upper and lower signs here and further refer to radiating and absorbing γ – quantum.

According to the formulas (8) it is easy to write an expression for energy γ – satellite, which corresponds to the transition $a \rightarrow b$:

$$E_\gamma = E_\gamma^{(0)} + \hbar k_\gamma v_0 \pm R_{OT} \pm (E_b - E_a), \qquad (9)$$

where the recoil energy of the molecule:

$$R_{OT} = (E_\gamma^{(0)})^2 / 2Mc^2. \qquad (10)$$

The specific quantum mechanical expressions to determine the probabilities of the corresponding cooperative processes (decay channels) are in details presented in Refs. [28-41]. It should be noted at once that in the case of diatomic (polyatomic) molecules the main interest is connected with studying the vibrational-nuclear and vibrational-rotational-nuclear transitions.

It is well known that purely electron-nuclear transitions associated with changes in the electronic state of a molecule are characterized by a very small probability (the corresponding probabilities are proportional to the square of the ratio m_e/M, where m_e – mass of electron, M – mass of a molecule), in this regard, the known Scilard-Chalmers effect is usually explained by the fact that the dissociation of the molecule during radiating or absorbing γ-quantum by the nucleus of the molecule is more likely to occur not due to the excitation of the electronic states of the molecule, but due to the direct rupture of the molecule in the ground electronic state.

It is easily to understand that only transitions between vibarational and rotational levels are of a great practical interest, including transitions to a continuous spectrum, accompanied by dissociation of molecules. As a rule, for such transitions the matrix element (4) has a standard form:

$$M_{ba} = \langle \Psi_b^*(R_1, R_2) | e^{-i\vec{k}_\gamma R_1} | \Psi_a(R_1, R_2) \rangle. \qquad (11)$$

The simplest model approach to the description of vibrational-rotational transitions in molecules is based on simple models of harmonic oscillator and rigid rotator [30,31,36]. Such models allow to qualitatively find out the main features of processes, however, quantitative theory should be based on more adequate methods of describing the structure of molecules.

In the harmonic oscillator approximation for a diatomic molecule, the wave function of the nuclei depends only on the change between the nuclear distances $(R - R_0)$:

$$\Psi(R_1, R_2) = (2^v v! \sqrt{\pi/\alpha})^{-1/2} \exp(-\alpha Q^2/2) H_v(\sqrt{\alpha Q}), \qquad (12)$$

where $\alpha = \omega/\hbar$, $Q = (R_1, R_2)\sqrt{m}$, $m = m_1 m_2/M$- the combined mass of a molecule, m_1 and m_2 - masses of nuclei 1 and 2, and the coordinate of nuclei 1 CM relatively to molecule CM is defined by the known relationship:

$$R_1 = -\frac{m_2}{M} R = -\frac{m_2}{M}\left(R_0 + \frac{Q}{\sqrt{m}}\right) = -\frac{m_2}{M} R_0 - (\frac{m_2}{m_1 M})^{1/2} Q \qquad (13)$$

Energy of a γ- satellite, which corresponds to the transition of the molecule from the vibrational state v_a to the state v_b, in the harmonic oscillator approximation is equal to (instead (9)):

$$E_\gamma = E_\gamma^{(0)} + \hbar k_\gamma v_0 \pm R_{OT} \pm \hbar\omega(v_b - v_a). \qquad (14)$$

In the rigid rotator approximation, the wave functions describing the motion of the nuclei of a molecule in a state with certain J and K, are eigenfunctions of the angular momentum:

$$\Psi(R_1, R_2) = Y_{JK}(\vartheta, \varphi), \qquad (15)$$

where angles ϑ and φ determine in the spherical coordinate system the vector of the mutual position of the nuclei:

$$R^0 = R_2^0 - R_1^0.$$

The matrix element (11) in this case is presented in the form:

$$M_{J_b, K_b, J_a, K_a} = \langle Y_{J_b, K_b}^*(\vartheta, \varphi)|\exp(i a_0 \cos\gamma)|Y_{J_a, K_a}(\vartheta, \varphi)\rangle, \qquad (16)$$

where γ is the angle between the vectors $R^0(\vartheta, \varphi)$ and $k_\gamma(\xi, \eta)$.

The exponent in (4) is usually decomposed by Bessel functions into a half-integer order (see details in Refs. [30-36])

$$\exp(i a_0 \cos\gamma) = 4\pi \sqrt{\frac{\pi}{2a_0}} \sum_{l=0}^{\infty} i^l J_{l+\frac{1}{2}}(a_0) \sum_{m=-l}^{+l} Y_{lm}(\vartheta, \varphi) Y_{lm}^*(\xi, \eta). \qquad (17)$$

Change in the rotational state of a molecule during radiation or absorption γ - quantum nucleus in a molecule is completely determined by the magnitude of the momentum of the amount of motion transmitted to the molecule:

$$\hbar a_0 = \hbar k_\gamma R_1^0 = (E_\gamma^{(0)}/c)(m_2/M)R^0 \tag{18}$$

Energy of γ-satellites that correspond to the transitions of a diatomic molecule from the state v_a, J_a to the state v_b, J_b, obviously is

$$E_\gamma = E_\gamma^{(0)} + \hbar k_\gamma v_0 \pm R_{or} \pm \hbar\omega(v_b - v_a) + B[J_b(J_b + 1) - J_a(J_a + 1)] \tag{19}$$

The general expression for the matrix element corresponding to the vibrational-rotational-nuclear transition can be written as:

$$M_{J_b,K_b,J_a,K_a}^{v_b,v_a} = (4\pi)^{1/2}[(2J_a + 1)(2J_b + 1)]^{1/2}(-1)^{K_b}$$

$$\sum_{l=|J_b-J_a|}^{J_a+J_b} i^l \{2l + 1\}^{1/2} \langle \Psi_{v_b} |(\pi/2a)^{\frac{1}{2}}J_{l+\frac{1}{2}}(a)| \Psi_{v_a} \rangle \tag{20}$$

$$\begin{pmatrix} J_a & J_b & l \\ 0 & 0 & 0 \end{pmatrix} \sum_{m=-l}^{+l} Y_{lm}^* \begin{pmatrix} J_a & J_b & l \\ k_a & -k_b & m \end{pmatrix},$$

where

$$a = (E_\gamma^{(0)}/\hbar c)(m_2/M)R_0 \ (1 + Q/[(m)^{1/2}R_0]. \tag{21}$$

The general expression for the probability of an vibrational-rotational nuclear transition from the state υ_a, J_a to the state υ_b, J_b can be written as:

$$P_{J_b,J_a}^{v_b,v_a} = (2J_b + 1) =$$

$$= \sum_{l=|J_b-J_a|}^{J_a+J_b} \{2l + 1\} \left| \Psi_{v_b} \left| \left(\frac{\pi}{2a)^{\frac{1}{2}}J_{l+\frac{1}{2}}(a)}\right) \right| \Psi_{v_a} \right|^2 \cdot \begin{pmatrix} J_a & J_b & l \\ 0 & 0 & 0 \end{pmatrix}^2. \tag{22}$$

In the case of vibrational motion in a theory claiming quantitative accuracy, naturally, wave functions for a certain value of the corresponding quantum number must be found from the Schrödinger equation with the corresponding realistic potential (potential energy curves).

The atomic and molecular computational code "Superatom and SuperMol" (version 93) is used to calculate the corresponding matrix elements, lifetimes (see details in Refs. [72-120]).

In Refs. [107-120] it has been developed a new precise quantum mechanical approach to calculating the potential energy curves, molecular constants, dipole moments, etc of diatomic molecules, which is based on a new version of the formally exact Rayleigh-Schrödinger perturbation theory (PT) with a ab initio model zeroth approximation and taking into account the exchange-correlation effects as the effects of the perturbation theory second and higher orders ones (including the polarization interaction of external quasiparticles through a polarized framework, or their mutual shielding, iterations of the mass operator, continuum pressure, etc.).

Alternative approach is given by the model potential scheme for determining the potential energy curves of a diatomic molecule, which is constructed as the sum of several curves corresponding to different internuclear distances [109,115]. Note that this approach, in addition to the goal of using in calculating the spectra of gamma transitions of the nucleus in a diatomic molecule involves the independent calculation of molecular constants. Indeed there are many other different models, which could be used for realization of the formulated task (e.g. [121-155]).

Tests performance

Test Option 1.

1). Give the key definitions in electronic , vibrational, rotational spectroscopy of molecules; Explaine the vibrational structure of electronic bands, describe the intensity distribution in cooperative electron-vibrational spectra.

2)/ Explain: i) interpratation of the vibrational structure of electronic bands ii) calculation of the potential energy curves of ground and excvited states iii) electronic spectra of diatomic molecules, iv) cooperative electron-vibrational -rotational spectra of molecules, v) the technical details of the computation code.

3). Explain numerical procedure for determination of the laser cooperative electron-vibrational -rotational spectra of molecules

4). To carry out the numerical algorythm for computing parameters of the laser cooperative electron-vibrational -rotational spectra of molecule $LiCs$. To perform its pracrical realization (using Fortran PS, Version 4.0; PC Code: "Supermolecule" (all necessary numerical parameters should be self-taken).

Test Option 2.

1). Give the key definitions in electronic , vibrational, rotational spectroscopy of molecules; Explaine the vibrational structure of electronic bands, describe the intensity distribution in cooperative electron-vibrational spectra.

2)/ Explain: i) interpratation of the vibrational structure of electronic bands ii) calculation of the potential energy curves of ground and excvited states iii) electronic spectra of diatomic molecules, iv) cooperative electron-vibrational -rotational spectra of molecules, v) the technical details of the computation code.

3). Explain numerical procedure for determination of the laser cooperative electron-vibrational -rotational spectra of molecules

4). To carry out the numerical algorythm for computing parameters of the laser cooperative electron-vibrational -rotational spectra of molecule $NaCs$. To perform its pracrical realization (using Fortran PS, Version 4.0; PC Code: "Supermolecule" (all necessary numerical parameters should be self-taken).

Test Option 3.

1). Give the key definitions in electronic , vibrational, rotational spectroscopy of molecules; Explaine the vibrational structure of electronic bands, describe the intensity distribution in cooperative electron-vibrational spectra.

2)/ Explain: i) interpratation of the vibrational structure of electronic bands ii) calculation of the potential energy curves of ground and excvited states iii) electronic spectra of diatomic molecules, iv) cooperative electron-vibrational - rotational spectra of molecules, v) the technical details of the computation code.

3). Explain numerical procedure for determination of the laser cooperative electron-vibrational -rotational spectra of molecules

4). To carry out the numerical algorythm for computing parameters of the laser cooperative electron-vibrational -rotational spectra of molecule $RbCs$. To perform its pracrical realization (using Fortran PS, Version 4.0; PC Code: "Supermolecule" (all necessary numerical parameters should be self-taken).

Test Option 4.

1). Give the key definitions in electronic , vibrational, rotational spectroscopy of molecules; Explaine the vibrational structure of electronic bands, describe the intensity distribution in cooperative electron-vibrational spectra.

2)/ Explain: i) interpratation of the vibrational structure of electronic bands ii) calculation of the potential energy curves of ground and excvited states iii) electronic spectra of diatomic molecules, iv) cooperative electron-vibrational - rotational spectra of molecules, v) the technical details of the computation code.

3). Explain numerical procedure for determination of the laser cooperative electron-vibrational -rotational spectra of molecules

4). To carry out the numerical algorythm for computing parameters of the laser cooperative electron-vibrational -rotational spectra of molecule $LiRb$. To perform its pracrical realization (using Fortran PS, Version 4.0; PC Code: "Supermolecule" (all necessary numerical parameters should be self-taken).

Test Option 5.

1). Give the key definitions in electronic , vibrational, rotational spectroscopy of molecules; Explaine the vibrational structure of electronic bands, describe the intensity distribution in cooperative electron-vibrational spectra.

2)/ Explain: i) interpratation of the vibrational structure of electronic bands ii) calculation of the potential energy curves of ground and excvited states iii) electronic spectra of diatomic molecules, iv) cooperative electron-vibrational - rotational spectra of molecules, v) the technical details of the computation code.

3). Explain numerical procedure for determination of the laser cooperative electron-vibrational -rotational spectra of molecules

4). To carry out the numerical algorythm for computing parameters of the laser cooperative electron-vibrational -rotational spectra of molecule KFr.. To perform its pracrical realization (using Fortran PS, Version 4.0; PC Code: "Supermolecule" (all necessary numerical parameters should be self-taken).

Test Option 6.

1). Give the key definitions in electronic , vibrational, rotational spectroscopy of molecules; Explaine the vibrational structure of electronic bands, describe the intensity distribution in cooperative electron-vibrational spectra.

2)/ Explain: i) interpratation of the vibrational structure of electronic bands ii) calculation of the potential energy curves of ground and excvited states iii) electronic spectra of diatomic molecules, iv) cooperative electron-vibrational - rotational spectra of molecules, v) the technical details of the computation code.

3). Explain numerical procedure for determination of the laser cooperative electron-vibrational -rotational spectra of molecules

4). To carry out the numerical algorythm for computing parameters of the laser cooperative electron-vibrational -rotational spectra of molecule NaK.. To perform its pracrical realization (using Fortran PS, Version 4.0; PC Code: "Supermolecule" (all necessary numerical parameters should be self-taken).

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