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 8 (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 "Molecular Optics and Spectroscopy", Part 8 (Training of PhD students of the specialty: 104 –"Physics and astronomy")

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Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline “Molecular Optics and Spectroscopy”, Part 8. (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: Molecular optics and spectroscopy. Application of electronic absorption spectra. Quantitative analysis by electronic absorption spectra

Topics: Molecular optics and spectroscopy. Application of electronic absorption spectra. Quantitative analysis by electronic absorption spectra
Топіки: Застосування електронних спектрів поглинання. Кількісний аналіз за електронними спектрами поглинання (ЗБ- Л2.8)

1 Introduction

The study of quantum processes of interaction of molecular systems, including molecules of an atmosphere, with intense electromagnetic radiation, in particular, the CO2 laser one, as well as the construction of quantitatively adequate models of energy exchange in mixtures of atmospheric molecules has traditionally attracted considerable interest [1-10]. This is largely due to the need to solve problems of monitoring the atmospheric environment using lidar (various laser) technologies.

It is well known that laser radiation has unique characteristics such as monochromaticity, directivity, coherence, and brightness. As a result, this provides the conditions for opening channels for the realization of numerous nonlinear effects (self-defocusing, self-focusing, self-channeling, pulse compression and decompression, soliton formation), in particular, along the propagation distance of the laser beam in the atmospheric medium. The physical aspects of these phenomena are qualitatively described in detail in Ref.[1-3]. In particular, according to Ref. [1-6], one should mention such resonant processes as a kinetic cooling effect, spectroscopic saturation effect, stimulated Raman scattering, different effects of laser chemistry as well as the non-resonant processes such as the non-resonant spectroscopic and thermochemical effects, electrostriction, the Kerr effect etc (other details can be found in Refs. [1-6]).

The classical laser sensing methods is mainly based on the processes of linear interaction of an electromagnetic (laser) radiation with the atmospheric gases and aerosol components of the atmosphere [1-10]. However, as it was shown in multiple investigations (c.g., [1-28]), there are a number of important problems and tasks, where the linear methods of sensing are ineffective both due to technical difficulties arising due to small interaction cross sections and because of fundamental physical limitations when these effects do not contain information about the desired medium parameters.

First of all, speech is about such tasks as remote elemental analysis of condensed matter of aerosols and underlying surface, determination of heavy metals and inert gas atoms content, detection of ultra-low concentrations of gas impurities and substance vapors with selective absorption coefficients cm^{-1}, and a number of other problems related, in particular, to diagnostics industrial pollution etc [1,5,6].

It is very important to remember about some fundamental aspects of the interaction of electromagnetic radiation with atoms and molecules of the atmospheric environment, especially in a case of the intense external field. Here it should be noted a nonlinear response of atoms and molecules. The obvious consequence of resonant interaction (in particular, absorption) of electromagnetic radiation (hereinafter, as a rule, will be coherent, that is, laser radiation) by molecular gases of the atmosphere is the quantitative redistribution of molecules by the energy levels of internal degrees of freedom. In turn, this will change the so-called gas absorption coefficient. Changing the population levels of the mixture of gases causes a disturbance of thermodynamic equilibrium between the vibrations of molecules and their translational motion, resulting in kinetic cooling of the environment. In this paper we present an advanced quantum-kinetic model for describing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture (with accounting for the nonlinear radiation transfer and further possible chemical conversion mechanisms too [7]).

2 Advanced quantum-kinetic model

The interaction of laser radiation with a mixture of atmospheric gases, leads to relatively complex processes of resonant excitation transfer, in particular, from CO_2 molecules to nitrogen molecules. As a result, the complex dielectric constant of the atmospheric medium will change, which will lead to a significant transformation of the energy of laser pulses in the gas atmosphere [1-5].

The dielectric constant depends on the intensity of the electromagnetic wave *I* as follows:

$$\varepsilon = \varepsilon(I) = \bar{\varepsilon}_0 + \varepsilon_N(I), \qquad (1)$$

$$I = \frac{c\sqrt{\varepsilon_0}}{8\pi}\left|\vec{E}\right|^2 \qquad (2)$$

where *c* is the speed of light, *E* is the electric field strength of the wave. When laser radiation interacts with atoms and molecules of atmospheric gases, there is also the so-called Kerr electronic effect, which arises due to the deformation of the electron density distributed by the field, almost immediately following the change of field, as well as the orientation effect of Kerr [3].

The relaxation time of this effect for atmospheric air under normal conditions is 10^{-13}s. This effect leads to the dependence of the dielectric constant on the field of the electromagnetic wave in the formula (1) of the form

$$\varepsilon_N = \varepsilon_2 |E|^2. \quad (3)$$

For Gaussian beams and plateau beams, the Kerr effect leads to the self-focusing of light, described in detail, for example, in [3, 8, 9, 11]. If the length of the nonlinear interaction (self-focusing) is a Gaussian beam with radius R_0

$$L_N = \frac{R_0}{\sqrt{\varepsilon_2 |E|^2}} = R_0 \left(\frac{8\pi \varepsilon_2}{c\sqrt{\varepsilon_0}} I \right)^{-1/2}, \quad (4)$$

then the realization of the effect on distance L_N is possible if the threshold intensity is determined as follows [3]:

$$I_{THR} \geq \frac{c\sqrt{\varepsilon_0}}{8\pi} \frac{R_0^2}{\varepsilon_2 L_p^2} \quad (5)$$

Here I_{THR}~10^{10} W·cm^{-2} for $R_0=0.1$ and $L_p=10^3$ m. If $L_p=10^5$ m, then I_{THR}~10^8 W·cm^{-2}. For infrared laser wavelength λ=10.6 μm, the critical autofocus ($L_p = L_d$) power is [1]:

$$P_{kr} = \pi R_0^2 I_{THR} = \frac{c\sqrt{\varepsilon_0}}{8k^2 \varepsilon_2} = 1{,}7 \cdot 10^{11} \quad (6)$$

One finds $P_{kr} = 1{,}7 \cdot 10^9$ W for λ=1,06 μm.

Further let us present an advanced quantum-kinetic model to describe the nonlinear-optical (spectroscopic) effect caused by the interaction of infrared laser radiation with a gas atmosphere and consider the quantitative features of energy exchange in a mixture of CO_2-N_2-H_20 atmospheric gases of atmospheric gases. It generalizes the known Gordin-Osipov-Khokhlov model [3]. The original version of our approach have been earlier presented in Refs. [11-13].

Typically, for the quantitative description of energy exchange and the corresponding relaxation processes in a mixture of CO_2-N_2-H_20 gases in the laser radiation field, one should first consider the kinetics of three levels: 10°0, 00°1 (CO_2) i v = 1 (N_2). In Figure 1 it is presented the original scheme of the lower vibrational levels of the CO_2, N_2, O_2, and H_2O molecules [3, 11, 12].

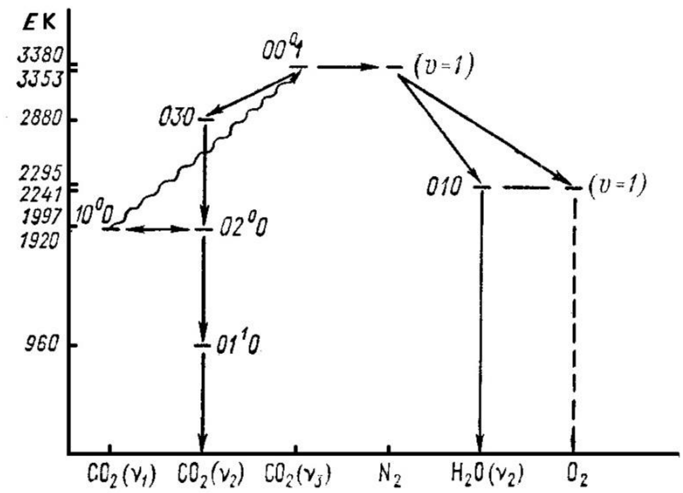

Figure 1 Scheme of the lower vibrational levels of the CO_2, N_2, O_2, H_2O molecules (see text)

The system of differential equations of balance for relative populations is written in the following form [14]:

$$\frac{dx_1}{dt} = -\beta(\omega + 2gP_{10})x_1 + (\beta\omega x_2 + 2\beta g P_{10})x_1^0 + F_N(x_1),$$

$$\frac{dx_2}{dt} = \omega x_1 - (\omega + Q + P_{20})x_2 + Qx_3 + P_{20}x_2^0 + F_N(x_2), \quad (7a)$$

$$\frac{dx_3}{dt} = \delta Q x_2 - (\delta Q + P_{30})x_3 + P_{30}x_3^0 + F_N(x_3).$$

Here,

$$x_1 = N_{100}/N_{CO_2},$$

$$x_2 = N_{001}/N_{CO_2}, \quad (7b)$$

$$x_3 = \delta N_{N_2}/N_{CO_2};$$ N_{100}, N_{001}

are the level populations 10°0, 00°1 (CO_2); N_{CO_2} is concentration of CO_2 molecules; δN_{N_2} is the level population v = 1(N_2); Q is the probability (s^{-1}) of resonant transfer in the reaction $CO_2 \rightarrow N_2$, ω is a probability (s^{-1}) of CO_2 light excitation, g = 3 is statistical weight of level 02°0, $\beta=(1+g)^{-1}$= ¼; δ is ratio of common concentrations of CO_2 and N_2 in atmosphere ($\delta = 3.85\cdot10^{-4}$); $F_N(x)$ – additional additive nonlinear term (see details in [13,14]; the elements of a chaos in the molecular systems are considered in many papers, e.g. [23-42]); x_1^0, x_2^0 and x_3^0 are the equilibrium relative values of populations under gas temperature T:

$$x_1^0 = exp(-E_1/T), \quad (8)$$

$$x_2^0 = x_3^0 = exp(E_2/T) \quad (9)$$

Values E_1 and E_2 in (1) are the energies (K) of levels 10°0, 00°1 (consider the energy of quantum N_2 equal to E_2); P_{10}, P_{20} and P_{30} are the probabilities (s^{-1}) of the collisional deactivation of levels 10°0, 00°1 (CO_2) and v = 1 (N_2). All calculations are performed with using the modified PC code “Superatom-Molecule” (the modified version 93 [13,14,43-56]).

Note that having obtained the solution of the differential equation system (17), one can further calculate the absorption coefficient of radiation by CO_2 molecules:

$$\alpha_{CO_2} = \sigma(x_1 - x_2)N_{CO_2}. \quad (10)$$

The σ in Eq. (20) is dependent upon the thermodynamic medium parameters according to [1]. The different estimates (eg, [1, 11]) show that for emission of the CO_2-laser the absorption coefficient:

$$\alpha_g = \alpha_{CO_2} + \alpha_{H_2O}. \quad (11)$$

is equal in conditions, which are typical for summer mid-latitudes α_g[H=0]=(1.1-2.6)·10^6 cm^{-1}, from which 0.8·10^6 cm^{-1} accounts for CO_2 and the rest – for the water vapour (data are from Refs. [1,3,13,14]) .

The resonance absorption of laser radiation by the molecules of the atmospheric mixture is obviously determined by the change in the population of the low-lying level 10°0 (CO_2), the population of the level 00°1 and vibration-translational relaxation (VT-relaxation), as well as intergenerational vibrational relaxation (VV'-relaxation). For the wavelength of infrared laser radiation (eg, CO_2 laser of 10.6μm), the duration of the corresponding pulses will satisfy the inequality $t_R \ll t_i < t_{VT}$,, where t_R, t_{VT} are the values of time, respectively, of the rotational and oscillatory relaxation.

In Ref. [12] there are presented the results of an accurate numerical calculations with using the accurately determined probabilities of P_{10}, P_{20} , P_{30} of deactivation due to the levels of 10°0, 00°1 (CO_2) and v = 1 (N_2), the probability of Q resonance energy transfer $CO_2 \rightarrow N_2$, the excitation probability ω pulse of CO_2 laser and other constants. The results of computing the relative absorption coefficient $\overline{\alpha}_{CO_2}$ (normalized to linear absorption coefficient) based on the solutions of the system (17) have been presented in Table 1.

Table 1. Temporal (μs) dependence of the relative resonant absorption coefficient (cm^{-1}) for rectangular (R), Gaussian (G) and soliton-like (S) laser pulses (intensity I, W/cm^2) altitude H = 10 km: A – model estimates [1]; B, C - our data

t μs	A $I=10^5$ R	A $I=10^6$ R	B $I=10^5$ R	B $I=10^6$ R	B $I=10^5$ G	B $I=10^6$ G	C $I=10^5$ S	C $I=10^6$ S
0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
1	0.48	0.12	0.46	0.12	0.41	0.11	0.43	0.10
2	0.34	0.08	0.32	0.07	0.26	0.04	0.29	0.05
3	0.41	0.27	0.37	0.19	0.31	0.18	0.34	0.19
4	0.48	0.35	0.44	0.29	0.37	0.26	0.39	0.27

The change in density is caused by heating or cooling the gas during the absorption of laser energy by a molecular gas. The bulk density of heat sources is easily expressed as follows (e.g. [1,2]):

$$q_T = \alpha_{H_2O} I + q_{T_{CO_2}}; \qquad (12)$$

$$q_{T_{CO_2}} = E_1 P_{10}(N_{100} - N_{100}^0) + E_2 P_{20}(N_{001} - N_{001}^0) E_2 P_{30}(N_{N_2} - N_{N_2}^0). \qquad (13)$$

As seen from (12) (see details in Refs. [1,2]), the first term in this expression describes the release of heat due to the absorption of light energy by water vapor, the second term determines the energy flux to the translational degrees of freedom due to vibrational relaxation CO_2 and N_2.

Using the obtained data one could determine that the effect of kinetic cooling of the CO_2 is determined by the condition (for Odessa region):

$$\alpha_{H_2O}^0 < \left(E_1/(E_2 - E_1)\right)\alpha_{CO_2}^0 = 1.51\alpha_{CO_2}^0 \qquad (14)$$

Note that Eq. (14) is sufficiently significantly different from early qualitative estimates [1,2,13]. The numerical parameters obtained allow us to further quantify the effects of kinetic cooling of CO_2, depending on the parameters of an atmosphere model and the laser radiation parameters [3]. According to Ref. [1,2,13,14] an effect of kinetic cooling disappears at a certain critical intensity of laser radiation.

This is due to the fact that at high radiation intensities, the energy flux from the translational degrees of freedom to the vibrational ones, which is responsible for the existence of the kinetic cooling effect, reaches its maximum value and ceases to depend on the power of the incident radiation. Starting from a certain critical power, gas heating will prevail over its cooling for any moment of time.

4. Conclusions

To conclude, we presented an advanced quantum-kinetic model for describing nonlinear optical effects due to the interaction of infrared laser radiation (CO_2 laser) with the atmospheric molecules mixture. An obvious consequence of the resonant interaction (in particular, absorption) of electromagnetic radiation by atmospheric molecules mixture is a quantitative redistribution of molecules over the energy levels of the internal degrees of freedom. This phenomenon quantitatively changes a gas absorption coefficient.

A change in the population levels of the gas mixture causes a violation of the thermodynamic equilibrium between the vibrations of the molecules and their translational motion and causes a nonlinear effect of the kinetic cooling of the atmospheric environment. We have presented the advanced calculational data on a temporal dependence of the relative resonant absorption coefficient for rectangular, Gauss and soliton-like laser pulses. It is clear that the time dependence of the relative resonance absorption coefficient of laser radiation by CO2 molecules differs for different laser pulses. The condition of realization of an atmospheric environment kinetic cooling is obtained and compared with available estimates.

The quantitative manifestation of the kinetic effect may vary for different atmospheric conditions, laser radiation pulse energetic and geometric parameters, and different values of atomic-molecular parameters [21-3, 12-15].]

Tests performance

Test Option 1.

1). Formulate the quantum-kinetic model for describing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture; Construct the master system of differential equations of balance for relative populations. Explain: i) the level populations ii) calculation of electronic-vibrational-rotational spectra of **diatomic molecule N2** iii) energy flux to the translational degrees of freedom due to vibrational relaxation CO_2 and N_2, iv) CO_2-laser the absorption coefficient;
2). To carry out the numerical algorythm for computing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture;. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Supermolecule").

Test Option 2.

1). Formulate the quantum-kinetic model for describing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture; Construct the master system of differential equations of balance for relative populations. Explain: i) the level populations ii) calculation of electronic-vibrational-rotational spectra of **diatomic molecule O2** iii) energy flux to the translational degrees of freedom due to vibrational relaxation CO_2 and N_2, iv) CO_2-laser the absorption coefficient;
2). To carry out the numerical algorythm for computing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture;. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Supermolecule").

Test Option 3.

1). Formulate the quantum-kinetic model for describing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture; Construct the master system of differential equations of balance for relative populations. Explain: i) the level populations ii) calculation of electronic-vibrational-rotational spectra of **diatomic molecule C2** iii) energy flux to the translational degrees of freedom due to vibrational relaxation CO_2 and N_2, iv) CO_2-laser the absorption coefficient;
2). To carry out the numerical algorythm for computing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture;. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule”).

Test Option 4.

1). Formulate the quantum-kinetic model for describing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture; Construct the master system of differential equations of balance for relative populations. Explain: i) the level populations ii) calculation of electronic-vibrational-rotational spectra of **diatomic molecule CO** iii) energy flux to the translational degrees of freedom due to vibrational relaxation CO_2 and N_2, iv) CO_2-laser the absorption coefficient;
2). To carry out the numerical algorythm for computing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture;. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule”).

Test Option 5.

1). Formulate the quantum-kinetic model for describing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture; Construct the master system of differential equations of balance for relative populations. Explain: i) the level populations ii) calculation of electronic-vibrational-rotational spectra of **diatomic molecule NO** iii) energy flux to the translational degrees of freedom due to vibrational relaxation CO_2 and N_2, iv) CO_2-laser the absorption coefficient;
2). To carry out the numerical algorythm for computing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture;. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule”).

Test Option 6.

1). Formulate the quantum-kinetic model for describing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture; Construct the master system of differential equations of balance for relative populations. Explain: i) the level populations ii) calculation of electronic-vibrational-rotational spectra of **diatomic molecule SO** iii) energy flux to the translational degrees of freedom due to vibrational relaxation CO_2 and N_2, iv) CO_2-laser the absorption coefficient;
2). To carry out the numerical algorythm for computing nonlinear optical effects due to the interaction of infrared laser radiation with the atmospheric molecules mixture;. To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule”).

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Methodical instructions
for practical work, test performance, distance learning of PhD students in the discipline “Molecular Optics and Spectroscopy”, Part 6.
(Training specialty: 104 - “Physics and Astronomy”; 01.04.05- “Optics and Laser Physics” and others)

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