STATE UNIVERSITY OF MOLDOVA

Consortium: **State University of Moldova, Institute for Information Society Development, "Bogdan Petriceicu Hasdeu" State University of Cahul**

DOCTORAL SCHOOL OF NATURAL SCIENCES

In manuscript form

C.Z.U.: **535.37:535.14:539.196(043.2)**

MUNTEANU ION

QUANTUM COOPERATIVE ACTION OF SHORT RADIATION PULSES WITH BIOMOLECULES IN THEIR PROPAGATION THROUGH METAMATERIALS WITH ITS APPLICATION IN DIAGNOSTICS, TREATMENT AND INACTIVATION OF PATHOGENS

131.01 - MATHEMATICAL PHYSICS

Summary of the PhD thesis in physical sciences

Chișinău 2025

The thesis was developed in the Laboratory of Quantum Optics and Kinetic Processes, Institute of Applied Physics, Moldova State University, Doctoral School of Natural Sciences.

Scientific Coordinator-

ENACHI Nicolae	Doctor of Physical and Mathematical Sciences, University Professor, Moldova State University

Composition of the Doctoral Committee:

GERU Ion	Doctor of Physical and Mathematical Sciences, University Professor, Corresponding Member of the ASM, Moldova State University - ***President of the Doctoral Committee;***
ENACHI Nicolae	Doctor of Physical and Mathematical Sciences, University Professor, Moldova State University**- PhD supervisor*;***
CIOBANU Nellu	Doctor of Physical and Mathematical Sciences, Associate Professor, "Nicolae Testemițanu" State University of Medicine and Pharmacy of the Republic of Moldova – ***reviewer;***
EVTODIEV Igor	Doctor of Physical and Mathematical Sciences, University Professor, University of Political and Economic Studies "C. Stere" USPEE – ***referent;***
VOVC Victor	Doctor of Medical Sciences, University Professor, "Nicolae Testemițanu" State University of Medicine and Pharmacy of the Republic of Moldova – ***reviewer;***

The thesis defense will take place on October 22, at 2:00 PM, during the Meeting of the Public Defense Committee of the Doctoral Thesis within the Doctoral School of Natural Sciences, USM.

Location – State University of Moldova, M. Kogălniceanu 65 A, block 3, room 332, MD-2009, Chisinau, Moldova.

The doctoral thesis and the abstract can be consulted at the National Library of the Republic of Moldova, the Central Library of the State University of Moldova (MD 2009, Chisinau, Alexei Mateevici 60), on the ANACEC website (http://www.anacec.md)

The abstract was sent on September 15, 2025

President of the Doctoral Committee
Doctor of Physical and Mathematical Sciences, University Professor, Corresponding Member of the ASM — **GERU Ion**

PhD supervisor
Doctor of Physical and Mathematical Sciences, University Professor — **ENACHI Nicolae**

Author: — **MUNTEANU Ion**

TABLE OF CONTENTS

CONCEPTUAL POINTS OF THE RESEARCH

The COVID-19 pandemic has profoundly impacted society globally, affecting public health and transforming people's way of life. To prevent the spread of the SARS-CoV-2 virus, measures such as physical distancing, mask-wearing, and vaccination have been adopted. UV radiation, a form of ultraviolet radiation, has proven effective in disinfecting air and surfaces, with the ability to neutralize bacteria and viruses, including SARS-CoV-2. However, its use requires caution, as direct exposure can seriously damage the skin and eyes.

According to the theory developed by the authors [1], irradiation with ultraviolet radiation, especially UV-C, which corresponds to wavelengths ranging from , is one of the most effective antiviral methods, constantly capturing the interest of researchers. They claim that UV-C radiation has the ability to neutralize a wide variety of pathogens, including microbes, viruses, bacteria, fungi, and yeasts.

The absorption of UV-C radiation by DNA biomolecules is mainly caused by electronic transitions of the nucleotide bases: Thymine (T), Adenine (A), Cytosine (C) and Guanine (G). Each of these elements absorbs UV-C radiation at distinct wavelengths, generating specific absorption spectra, where the maximum absorption points for these DNA bases are found around ~265 nm [2].

The use of pulsed UV-C radiation is an innovative method, based on short and intense pulses, which increase the efficiency of inactivating microorganisms compared to continuous UV-C sources. In addition to damaging microbial DNA, this technique can generate additional photochemical effects, amplifying the neutralization process. Thus, the technology is effective in disinfecting air and surfaces, destroying the DNA/RNA structure of microorganisms, including bacteria, viruses and fungi, and preventing their ability to reproduce or cause infections.

Recently, the development of disinfection technologies for pandemic risk management has attracted the attention of researchers. An innovative approach involves the use of advanced optical manipulation techniques to inactivate pathogens. This includes analyzing the resistance of microorganisms and optimizing the decontamination process depending on the frequency and duration of light pulses. Some methods use effects such as "optical tweezers" in areas of intense radiation, especially with UV-C pulses, or apply centrifugal effects on rotating particles, such as aerosols or pathogens. These processes are based on the differences between the refractive indices of microorganisms and their environment, allowing them to be attracted to areas of more intense radiation, due to the "optical tweezers" effect. To increase the efficiency of pathogen inactivation devices, nonlinear cooperative

interactions between microorganisms, in the processes of photon absorption and emission, have been studied. A theoretical model, inspired by the Raman effect in quantum optics, shows that the dimerization process in DNA/RNA is significantly influenced by the intensity of UV-C radiation, suggesting a quantum microscopic phenomenon in the interaction with DNA. The Born-Oppenheimer approximation is a key principle in molecular quantum mechanics [3], which separates the motion of nuclei from that of electrons in a molecular system. It is crucial for the study of the interaction of UV-C radiation with DNA, in the dimerization of pyrimidine bases (thymine and cytosine). The intensity of the UV-C field changes the position of the nuclei during scattering, facilitating the tunneling of electrons between potential wells, which stimulates coherent nuclear vibrations and modifies the DNA. To explain the inactivation of pathogens by scattered UV-C radiation, which coherently eliminates the electronic subsystem, the Born-Markov approximation is used. This describes how UV-C radiation effectively neutralizes microorganisms by coherently eliminating the electronic subsystem.

The main goal of the work lies in the title of the thesis and consists in increasing the efficiency of pathogen inactivation equipment as a result of the cooperative quantum action of short pulses of UV-C radiation with biomolecules during their propagation among the elements of the metamaterial.

Research objectives:

1. Research on the specifics of the interaction of pulsed/continuous UV-C radiation according to the literature. Highlighting some disadvantages related to its penetration inside the translucent fluid.
2. Investigation of the possibilities of penetration of UV-C radiation inside the translucent (non-transparent) fluid using quartz fibers or beads that allow the wave to propagate inside it.
3. Estimation of the increase in the contact area of a metamaterial formed by fiber or bead subsystems when packing them, the impact of this estimate on the efficiency of inactivating pathogens.
4. Description of the mechanism of influence of the UV-C pulse duration resulting from the nonlinear interaction of biomolecules with radiation.
5. Research on the formation of molecular dimers in biomolecules (DNA, RNA) using the Born-Oppenheimer model adjusted to the external electromagnetic field. Influence of the fast electronic system on the displacement of nuclei under the action of coherent radiation.

6. Estimation of the possibilities of repackaging metamaterials and the effects of pathogen rotation among these metamaterials in the development of new equipment with increased decontamination efficiency.

Research hypothesis:

The use of pulsed UV-C radiation, in correlation with the principles of the Born–Oppenheimer model, allows for the optimization of the pathogen DNA dimerization process, and the integration of metamaterials in decontamination devices improves the efficiency of inactivation of microorganisms through precise control of radiation propagation. This hypothesis assumes the following:

-The efficiency of pulsed UV-C radiation in inducing pathogen DNA dimerization for inactivation.

-The application of the Born–Oppenheimer model in the analysis of the interaction of UV-C radiation with biomolecules, separating the electronic and nuclear motion to better understand the physicochemical mechanisms involved.

-The role of metamaterials in improving the manipulation and targeting of UV-C radiation in modern decontamination devices, increasing their effectiveness.

Synthesis of the research methodology and justification of the chosen research methods:

This research is of both theoretical and experimental type, combining theoretical models based on the Born–Oppenheimer model and the tweezer effect, as well as experimental methods for testing the inactivation of pathogens found among the elements of metamaterials penetrated by pulsed UV-C radiation. These theoretical and experimental methods involve:

-modeling the interaction of pulsed UV-C radiation with the DNA of biomolecules using the Born–Oppenheimer model.

-energy transfer of UV-C radiation on DNA.

-stability and mechanism of formation of thymine dimers.

-analysis of how concentrated electromagnetic fields can influence the structure of microorganisms and the propagation of UV-C radiation.

Justification of the chosen methods:

-The Born–Oppenheimer theoretical model provides a fundamental basis for understanding mechanisms at the molecular level. -Metamaterials and the tweezer effect are investigated to improve the precision and efficiency of decontamination devices, bringing technological innovation. -Experimental methods allow for the practical validation of the efficiency of pulsed UV-C in inactivating pathogens and DNA modifications; The above-mentioned methods, being present in modern physics research carried out in recent times, allow solving many problems related to the

efficient inactivation of pathogens from different environments upon their interaction with UV-C radiation.

Solved scientific problem:

A mechanism for efficient inactivation of microorganisms was highlighted based on theoretical and experimental research taking into account their correlation, as well as the development of a process for decontamination of pathogens accelerated in rotational motion among the metamaterial elements under the influence of pulsed UV-C radiation.

Main scientific results submitted for support:

1. Superior efficiency of pulsed UV-C radiation, performance of pulsed UV-C sources compared to continuous ones: Pulsed UV-C radiation technology, based on short and intense exposures, demonstrates increased efficiency in inactivating pathogens, significantly reducing the duration of the sterilization process compared to continuous UV-C sources, which require prolonged exposure times.

2. The Born-Oppenheimer approximation, applied in the context of DNA dimerization induced by UV-C radiation, allows modeling of molecular dynamics by separating the motion of atomic nuclei from that of electrons, facilitating the description of the dimerization process through a nonlinear model of interaction between DNA molecular subsystems and laser pulses.

3. Use of quartz metamaterials: The integration of translucent quartz metamaterials into pulsed UV-C systems improves light penetration, which leads to a substantial increase in the pathogen inactivation rate and a reduction in the exposure time required for decontamination.

4. Modern advanced decontamination equipment using short-pulse UV-C and translucent metamaterials for optimized efficiency in pathogen inactivation: The technology based on short-pulse UV-C radiation, integrated with translucent quartz metamaterials, optimizes light penetration and irradiation dose control, ensuring rapid and effective pathogen inactivation.

Approval of the results obtained

The basic results of the work were presented and discussed at **2 international conferences:** IEEE International Conference on e-Health and Bioengineering EHB 2022 - 10-th Edition, 17-19 November 2022, Hybrid Conference, Iasi – Romania, IEEE Conference Advanced Topics on Measurement and Simulation (ATOMS), Constanta. Romania, and **4 national conferences:** Technical-scientific conference of students, master's and doctoral students, April 5-7, 2023, Chisinau, International scientific-practical conference "Education through research for a prosperous society", 11th edition, March 16-17, 2024, National Conference with International Participation: NATURAL SCIENCES IN THE DIALOGUE OF GENERATIONS, 7th edition, September 12-13, 2024, Chisinau, Volume I, Chisinau, Scientific-practical conference "ADVANCED PHYSICAL TECHNOLOGIES WITH THE APPLICATION OF UVS IN MONITORING AND MODELING OF ENVIRONMENTAL FACTORS", 5th edition, November 8, 2024, and **10 international / national invention fairs**: INVENTICA 2022, Iași, Romania, PRO INVENT 2022, October 26 - 28, 2022, Romania, EUROINVENT 15th European Exhibition of Creativity and Innovation, Iasi, Romania, May 11-13, 2023, "INVENTICA 2023" Iasi, PROINVENT, 21st edition, October 25-27, 2023, CLUJ-NAPOCA, International Exhibition of Inventions and Innovations "Traian Vuia" 2023, Timișoara, International Exhibition INVENTCOR – 5th edition, April 4-6, 2024, Deva, International Exhibition of Inventions and Innovations "Traian VUIA", June 13-15, 2024, Timișoara, European Exhibition of Creativity and Innovation EUROINVENT, June 6-8 2024, Iași, International Specialized Exhibition INFOINVENT 2023 XVIII Edition, November 22-24.

Publications on the topic of the thesis

In total, the results on the topic of the thesis are published in 15 scientific papers, of which 4 articles in international journals listed in Web of Science and SCOPUS (The European Physical Journal - Plus (EPJ Plus), MDPI Materials, European Biophysics Journal Springer, IEEE Xplore), 1 article in national journals (Studia Universitatis Moldaviae, Revista științtă a Universității de Stat din Moldova, 2024, no. 1(171), 109-115.CZU: 535.37:616.314-089. (Category B)), 5 scientific papers in journals from other databases accepted by ANACEC, 5 reports/theses of communications at congresses, conferences, symposia, in collections, 3 patents. Of these, 1 patent, 2 articles and 2 abstracts are published without co-authors.

Keywords:

UV-C radiation, short pulses, metamaterials, dimerization, decontamination.

THESIS CONTENT

The introduction underscores the significance and timeliness of the topic, clearly articulating the relevance of the research problem. It defines the overarching purpose and specific objectives of the study. The choice of methodology is justified in alignment with the stated purpose, with the selected methods thoroughly rationalized.

Chapter One, *"Development of Decontamination Technologies Using Short Light Pulses and Metamaterials"* provides an analysis of the current state of research on innovative technologies for pathogen decontamination. Advanced decontamination is a strategic field with applications in healthcare, the food industry, security, and ecology. Among emerging methods, the use of short light pulses and metamaterials stands out, promising enhanced efficiency in neutralizing microorganisms in various environments.

UV-C radiation (200–280 nm) is effective in inactivating microorganisms by damaging their DNA and RNA, preventing replication [1,2]. Recent studies confirm its effectiveness against SARS-CoV-2, with doses of 3.7 mJ/cm² achieving over 3-log inactivation and 16.9 mJ/cm² ensuring complete inactivation [3]. Efficiency depends on factors such as radiation intensity, exposure duration, and the surrounding environment. Decontamination efficiency is quantified by the logarithmic reduction of pathogens, calculated using the formula:

$$\eta = \left(1 - \frac{N_f}{N_i}\right) \times 100, \tag{1}$$

where η is the percentage of inactivation, and N_i and N_f are the initial and final numbers of pathogens, respectively. The required UV-C radiation dose varies depending on the microorganism, ranging from [value] for coronaviruses to [value] for adenoviruses [4,5]. To determine the number of pathogens remaining after decontamination, the following equation is used:

$$LOG10_{Inactiv.Pathogen} = -\log_{10}(1 - \frac{I_{patogen}}{100}). \tag{2}$$

Formula (2) calculates the number of pathogens remaining after decontamination has occurred. For example, if a surface (let's assume a table) with a colony of 1 million viruses undergoes decontamination, an inactivation rate of 1-log or 90% will leave 100,000 viruses behind. Table (1) presents the various connotations:

Table 1. Accurate measurement of pathogen reduction rate

LOG/Rate	1-log	2-log	3-log	4-log	5-log	6-log
Inactivation rate (%)	90%	99%	99,9%	99,99%	99,999%	99,9999%
Viruses left over from 1 million	100.000	10.000	1.000	100	10	1

According to the theory in [6], the amount of viral inactivation achieved for a given UV radiant flux (irradiance) is easily described using the following first-order decay equation

$$N_t = N_0 \times e^{-Z \cdot E \cdot t}, \tag{3}$$

where: N_0 and N_t are the number of viable viral particles (virions) at time zero and after t seconds, respectively; k is the UV susceptibility (sensitivity) constant for the virus (m²/J); E is the radiant flux (irradiance) (W/m²); and t is the time in seconds. The UV irradiation dose received by the virus can be expressed by the relationship:

$$D = E \times t, \tag{4}$$

where: D is the UV irradiation dose, expressed in (J/m²). By combining equations (3) and (4), the value for the susceptibility constant Z can be obtained:

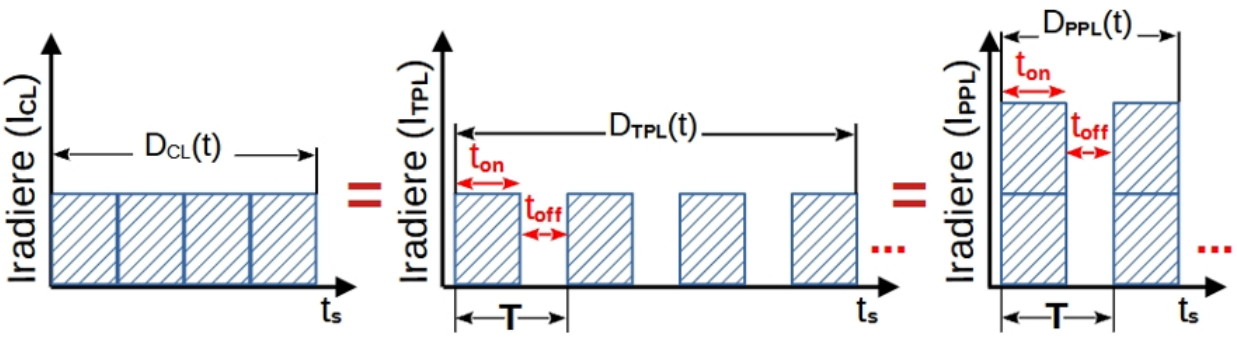
$$Z = -\frac{1}{D} \times \ln\left(\frac{N_t}{N_0}\right) = -\frac{1}{D} \times \ln(f), \tag{5}$$

where f is the survival fraction. The fact that the relationship between the UV dose and the natural logarithm of the survival fraction is linear for most pathogens (5) indicates that the state of any pathogen exposed to UV radiation can be described using Z, regardless of the sufficiently applied UV dose. Once the value of Z is determined, the behavior of the pathogen exposed to a specific UV radiation dose can be predicted with high accuracy in any situation. Pathogens with high Z values are more susceptible to damage caused by UV radiation, while those with low Z values are harder to inactivate [6].

UV-C sources, such as lamps and lasers, differ in the nature of their emissions—continuous or pulsed. UV-C radiation, particularly in pulsed mode, plays a crucial role in efficient microorganism decontamination due to its high peak intensity and the ability to precisely adjust pulse parameters. Microbial inactivation depends on the dose D, exposure time t, and applied irradiance. UV-C LEDs can operate in continuous mode (CL), time-pulsed mode (TPL), or power-pulsed mode (PPL), as illustrated in Fig. 1. The applied radiation dose is determined by the relationship:

$$D_{CL}(t) = \int_0^{t_{CL}} I_{CL} \times t \, dt. \tag{6}$$

Fig. 1 illustrates the configuration of various UV-C LED light techniques used for microorganism decontamination. To highlight that in all three cases the same irradiance I_{CL} is applied, the shaded area is divided into four sectors.



a) **b)** **c)**

Fig. 1. UV-C LED emission techniques. a) Continuous light (CL). b) Time-pulsed light (TPL). c) Power-pulsed light (PPL).

As observed, Fig. 1a presents the spectral distribution over a period of time for the continuous emission mode of energy (photons), while for pulsed light, two types of modes are shown: Mode 1 (Fig. 1b) and Mode 2 (Fig. 1c), which differ in the dose established at different frequencies or, in other words, the number of cycles per second.

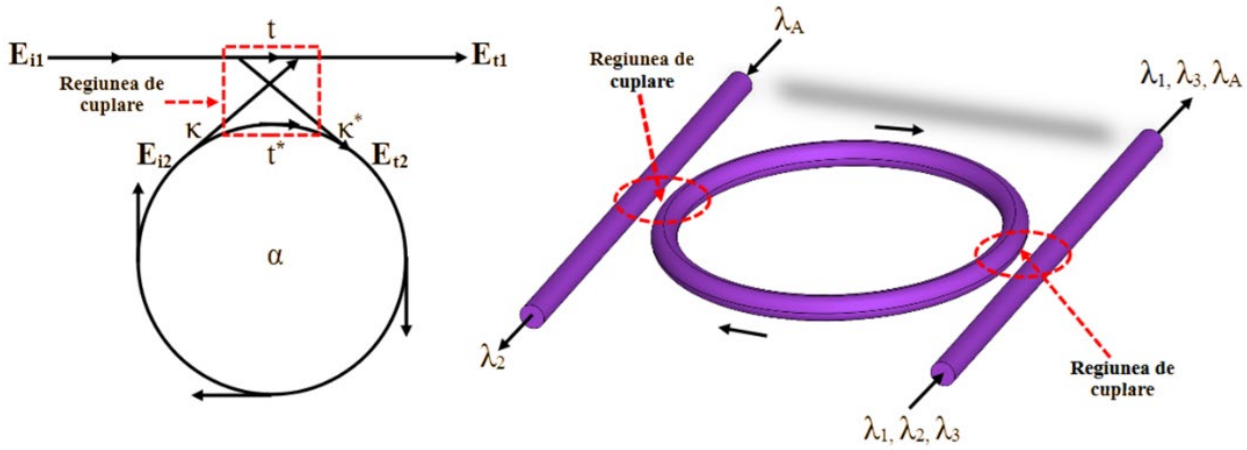
Pulsed light offers a significant advantage over continuous light, including not only the ability to adjust intensity by modifying the frequency but also the flexibility in setting the pulse duration and duty cycle. This approach enables precise control of optical parameters, including exposure time and pulse intensity, ensuring efficient and accurate energy application to exposed surfaces. The pulse shape can be described by a Gaussian function:

$$I(t) = I_0 \exp\left(-\frac{(t-\mu_0)^2}{2\sigma^2}\right), \tag{7}$$

where $I(t)$ is the pulse intensity at time t, I_0 is the maximum intensity, μ_0 is the pulse center in time (the moment when power is maximum), and σ is the pulse width. Experiments show that short pulses (5 ns) reduce the inactivation time to a few seconds, compared to the minutes required for continuous sources [7].

The whispering gallery mode phenomenon, initially observed by Rayleigh, forms the basis of nonlinear resonator models, where electromagnetic waves propagate along the resonator's surface with reduced intensity loss compared to free space.

Figure 2 presents two nonlinear resonator models described in [8, 9]: (a) a single-waveguided ring resonator and (b) a ring resonator with two guided waves. The unidirectional coupling in model (a) involves a ring resonator of radius R interacting with a waveguide in the coupling region λ_A, generating the transmitted fields E_{t1} and E_{t2}. Model (b) extends this configuration by incorporating bidirectional coupling with two waveguides, characterized by coupling regions $\lambda_1, \lambda_2, \lambda_3, \lambda_A$ that facilitate complex field interactions.



a) **b)**

Fig. 2. a) Model of a ring resonator with a single waveguide. b) Model of a ring resonator with two waveguides.

The integration of capillary fibers and dielectric spheres enhances the efficiency of optical biomolecule capture by exploiting whispering gallery modes, a principle widely applied in integrated ring resonators for advanced biosensor applications.

If the coupling is limited to waves traveling in one direction (with no reflection), and the total input power equals the output power, then the coupling can be described using two constants, κ and τ, respectively, and a unitary scattering matrix:

$$\begin{pmatrix} E_{t1} \\ E_{t2} \end{pmatrix} = \begin{pmatrix} t & k \\ t^* & k^* \end{pmatrix} \begin{pmatrix} E_{i1} \\ E_{i2} \end{pmatrix}, \tag{8}$$

where, E_{t1}, E_{t2} are the input powers of the traveling waves in this coupling, and P_3 and P_4 are the output powers, respectively. The coupling matrix is unitary when it satisfies the relationship:

$$\left|k^2\right| + \left|t^2\right| = 1. \tag{9}$$

he specific form of S is not particularly necessary, as it depends on the specific coupling mechanism used. Equation (8) and the condition for the coupling matrix to be unitary are complemented by the ring circulation condition. Thus, the transmission around the ring is given by the following relationship:

$$E_{i2} = \alpha e^{i\theta} E_{t2}, \tag{10}$$

where α is the internal circulation factor, a real quantity, and for zero internal losses, a = 1. From equations 8, 9, and 10, we obtain:

$$E_{t1} = \frac{-\alpha + te^{-i\theta}}{-\alpha t^* + e^{-i\theta}}; \qquad E_{i2} = \frac{-\alpha k^*}{-\alpha t^* + e^{-i\theta}}. \tag{11}$$

The signal passing through the resonator from the input waveguide is given by:

$$\left|E_{t1}\right|^2 = \frac{\alpha^2 + \left|t\right|^2 - 2\alpha\left|t\right|\cos(\theta + \varphi_t)}{1 + \alpha^2\left|t\right|^2 - 2\alpha\left|t\right|\cos(\theta + \varphi_t)}, \tag{12}$$

where, $t = \left|t\right|\exp(\mathrm{i}\varphi_t)$, while the total circulating power is:

$$\left|E_{i2}\right|^2 = \frac{\alpha^2(1 + \left|t\right|^2)}{1 - 2\alpha\left|t\right|\cos(\theta + \varphi_t) + \alpha^2\left|t\right|^2}. \tag{13}$$

Most of the interesting characteristics of this resonator appear near resonance, where $(\theta + \varphi_t) = m2\pi,$ where m is an integer. In such a situation, at resonance, equations (12, 13) can be written as follows:

$$\left|E_{t1}\right|^2 = \frac{\left(-\alpha^2 + \left|t\right|\right)^2}{\left(1 - \alpha\left|t\right|\right)^2}; \qquad \left|E_{i2}\right|^2 = \frac{\alpha^2\left(1 - \left|t\right|\right)^2}{\left(1 - \alpha\left|t\right|\right)^2}. \tag{14}$$

The first part of equation (14) is of particular interest, as it shows that when the transmitted power vanishes (is zero) $\left|E_{t1}\right|^2 = 0$ at a coupling value $\alpha = \left|t\right|$, known as "critical coupling," this is due to the internal losses (represented by a) being equal to the coupling losses (represented by $\left|t\right|$). The critical coupling condition is an essential property of waveguides coupled to resonators. It refers to the situation where the internal losses of the resonator and the coupling losses of the waveguide are equal in a corresponding resonator-waveguide system [10]. At this point, the resulting transmission at the waveguide output becomes zero at the resonance frequency.

Technologies based on short light pulses and metamaterials are revolutionizing decontamination methods by providing fast, efficient, and environmentally friendly solutions. In the future, the integration of these technologies could eliminate the need for hazardous chemical substances, offering a safer environment in critical fields such as medicine, the food industry, and environmental protection.

Chapter two *"Experimental methodology. Coherent action of pulsed UV radiation with biomolecules"* explores the interaction of UV-C radiation with matter, highlighting the vulnerability of pathogens (bacteria, viruses, fungi) to specific doses of radiation, which affect essential cellular components. The lethal effect of UV radiation on microorganisms is analyzed, with an emphasis on the dimerization of pyrimidine bases (thymine and cytosine) in DNA and RNA, as a direct result of the absorption of UV photons.

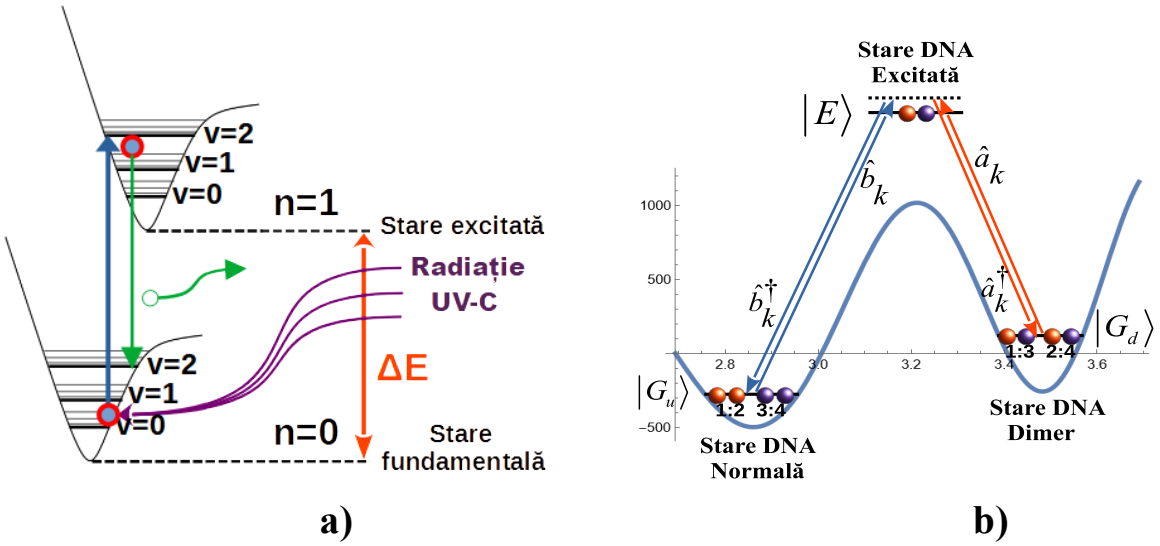


Fig. 3. a) Absorption of UV-C radiation by the molecule with its transition on energy levels. b) Formation of thymine dimers caused by absorption of UV-C radiation.

The interaction of electromagnetic radiation with matter is based on the absorption or emission of characteristic radiation (Fig. 3). Molecular transitions from the ground state to the excited state are described mathematically by the relationship of the absorbed photon energy: $\Delta E = E_e - E_f = \frac{hc}{\lambda}$, where, wavelength $\lambda = \frac{hc}{\Delta E}$, frequency $\nu = \frac{\Delta E}{h}$, E_f and E_e are the energy of the ground and excited states, h – Planck's constant, c – the speed of light in a vacuum and ν – the frequency of the emitted radiation.

The quantum description of the transition is nothing more than the absorption of UV-C radiation is described by the interaction of the electromagnetic field of the photon with the electric dipole of the molecule. The transition probability is given by Fermi's golden rule: $W_{i\to f} = \frac{2\pi}{\hbar} |\langle \psi_f | \hat{H}_{\text{int}} | \psi_i \rangle|^2 \rho(E_f)$, where ψ_i, ψ_f are the wave functions of the initial and final states, $\hat{H}_{\text{int}}$ is the interaction Hamiltonian, $\rho(E_f)$ is the density of states at the final energy, and $\hbar = \frac{h}{2\pi}$. For an electromagnetic field the interaction Hamiltonian is the vector product between the electric dipole moment of the molecule $\vec{\mu}$ and the electric field of the radiation $\vec{E}$, or $\hat{H}_{\text{int}} = -\vec{\mu} \cdot \vec{E}$. The matrix element of the dipole is: $\langle \psi_f | \vec{\mu} | \psi_i \rangle = \int \psi_f^* \vec{\mu} \psi_i \, dV$, and at the same time this integral determines the transition probability. For example, if $\langle \psi_f | \vec{\mu} | \psi_i \rangle = 0$, transition is forbidden (selection rules).

The technique of pulsed UV-C irradiation with the help of a laser inactivates viruses by destroying DNA, with the formation of T=T dimer bonds. Another approach in this

regard is that, after irradiation, the virus begins to oscillate, in one way or another it tends to behave like phonons in the solid lattice, and from the point of view of quantum mechanics the free Hamiltonian of the molecular system can be represented according to the Born–Oppenheimer (B-O) approximation $\hat{H}_e\hat{H}_n$, where $\hat{H}_e$ is the energy of the binding electrons interacting with the laser field upon excitation, and $\hat{H}_n$ is the energy of the nuclear subsystem of the biomolecule, which can be represented by a set of nonlinear oscillators with generalized coordinate $X_i = \{X_1, X_2, ..., X_n\}$. We will simplify the problem by investigating only the behavior of a nucleus or set of nuclei in the region r of the molecule.

$$\hat{H}_n = \frac{M}{2}\{\frac{d^2X}{dt^2} + \Omega^2 X^2 - 2\chi X^4 / M\}. \quad (15)$$

Here, we consider a single vibration mode of the virus, where M is the effective mass of the viral molecule (DNA protein segment), Ω is the vibration frequency of the pathogen's molecular nuclei, χ characterizes the anharmonic parameter of the vibration mode. The first term in the Hamiltonian (15) represents the possible kinetic energy states of the particle, while the second and third terms represent the corresponding possible potential energy states. To better understand this vibration mode, we consider the situation of the string in which the notion of mass density is introduced $\rho = \sum_i M_i / v$, where M_i is the mass of a subdivision of the molecule in vibration (e.g. Carbon, Oxygen, Nitrogen etc...), and v is the volume of this molecular subdivision. So, by M in expression (15) we mean $\rho \times v$ as in the case of the rope.

Because the electronic subsystem is fast compared to the nuclear subsystem of biomolecules, $\tau_e / \tau_n \sim m / M < 1$, it is necessary to solve the quantum problem of excitation of the electronic subsystem, considering that the atomic subsystem of nuclei is slow and can be considered fixed. The energy of this interaction with the electronic subsystem can be represented as the sum of the electronic dipoles interacting with the laser field $\hat{H}_I = -P^*(r, X)E(r)$, where $P^*(r, X)$ și $E(r)$ is the polarization and the field in the region of the pathogen biomolecule. Since the process is Raman type, we can eliminate the virtual levels of the electronic subsystem as exposed in [13]. However phenomenologically we could decompose the polarization by the field as presented in [14]:

$$P^*(r, X_s) = P_0 + \alpha_j(X_s)E_j^*(r) + + \alpha_{j,l}(X_s)E_j^*(r)E_l^*(r) + ... + .. \quad (16)$$

In Raman resonance only the second term contributes to the nonlinear vibrational excitations of the molecular nuclei. Moving to longer times the electronic polarization can be decomposed in series according to the X coordinates of the nuclear subsystem

of the biomolecule. The vibrational mode of a pathogenic biomolecule (virus, bacterium, fungus, etc..) excited by the UV laser can be written explicitly representing in the Taylor series described by the expression below:

$$\alpha_j(X) \simeq \alpha_j(0) + X\partial\alpha_j(0)/\partial X\,, \tag{17}$$

where the set of coordinates X represents the degrees of freedom of the nuclei in nonlinear vibration [15]. Considering that according to Newton's second law the product of mass and acceleration must be equal to the force, $M\ddot{X} = -\frac{\partial}{\partial X}\{H_n + H_i\} - \gamma\dot{X}$, thus the following equation is obtained:

$$\frac{\partial^2 X}{\partial^2 t^2} + \gamma\frac{\partial X}{\partial t} + (\Omega^2 - 4\chi X^2)X = F_{ext}/M = [\partial\alpha_j(0)/\partial X]E_j^*(t)E(t)/M\,, \tag{18}$$

where γ is the damping parameter, $\gamma \times v$ vibration damping force and $\Omega = \sqrt{\kappa/M}$ represents the anharmonic constant of the oscillator. The right-hand side of expression (18) corresponds to the impulsive driving force produced by the excitation laser on the slow nuclear subsystem of the biomolecule and can be calculated as the derivative with respect to the generalized coordinates of the nuclear subsystem $F(t) = -\partial\hat{H}_I/\partial X$. Deriving the expression for X α_j we obtain the expression below for the force

$$F_{ext} = [\partial\alpha_j(0)/\partial X]E_j^*(t)E(t)\,, \tag{19}$$

where expression, $E_j^*(t)E(t)$ represents the product of the electric vector at the pumping and Stokes frequencies so that this product can be represented by the difference in frequencies at the exponent $E_j^*(t)E(t) \sim \exp[(\omega_p - \omega_s)] + H.c.$ Here it must be considered that the difference between the pumping frequency and the Stokes frequency must be approximately equal to the natural frequency of the molecular oscillator formed by nuclei, $\Omega_0 \approx \omega_p - \omega_s$. The polarizability has a static part that induces elastic Rayleigh scattering and is modulated by the oscillatory displacement. For small damping, the displacement is $X(t) = X_0 e^{-i\gamma t} sin\Omega t$. Amplitude of displacement X_0 with respect to the equilibrium position of the virus is given by:

$$X_0 = \frac{\sqrt{\pi}}{2}\frac{n\tau}{ck\omega}a_0' E_0 e^{-(\Omega_0\tau/2)^2}\,. \tag{20}$$

Here E_0 and τ are the peak intensity and pulse width of the laser, respectively, given by the relationship:

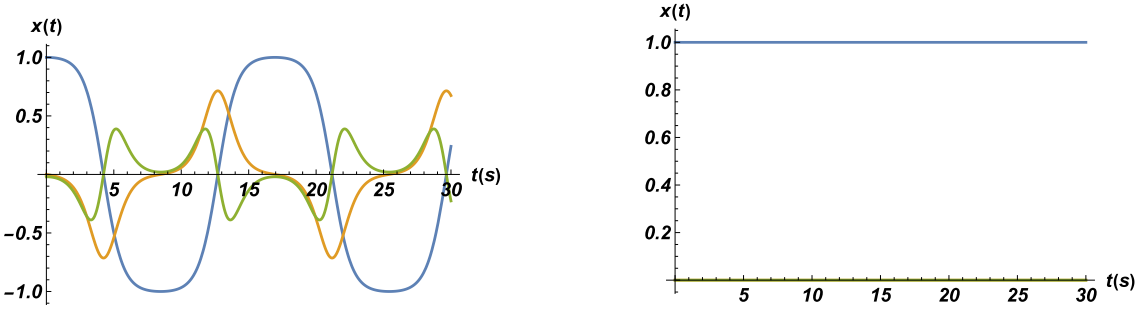
$$E_L(t) = E_0 exp\left[-\left(\frac{t}{\tau}\right)^2\right]. \tag{21}$$

α_0 is the polarizability derivative proportional to the Raman scattering amplitude, n is the refractive index, the speed of light, and the permittivity of the dielectric medium.

Let's introduce the value of the external force $F_{ext}/M = \frac{\alpha' E_p^*(0)E_s(0)}{M}\exp[i(\omega_p - \omega_s)t]$ where $\Omega_0 = \omega_p - \omega_s$, and $\Delta = \Omega - \Omega_0 \to 0$ is called the deviation from resonance $F_{ext}/M = \alpha' E_p^*(0)E_s(0)\exp[i\Omega_0 t], \alpha' = [\partial\alpha_j(0)/\partial X]$. In accordance with this concept, equation (18) becomes the following:

$$\frac{\partial^2 X}{\partial t^2} + \gamma\frac{\partial X}{\partial t} + [\Omega^2 - 4\chi X^2]X = \frac{\alpha' E_p^*(0)E_s(0)}{M}\exp[i\Omega_0 t] \qquad (22)$$

Using the Wolfram Mathematica software, we built the graph of the function $\left[\left\{x''[t] + \left(W - 4*k*x[t]\text{^}2\right)*x[t] == 0, x[0] == 1, x'[0] == 0\right\}, x, \{t, 0, 30\}\right]$, to understand whether there is and what the value of the critical point would be where the biomolecule no longer oscillates.



a) **b)**

Fig. 4. a) Up to the critical point $\chi = 0,25$ there is vibration of the molecule b) $\chi > 0.25$ the molecule is broken, it no longer oscillates

In the first order of perturbation theory we neglect the nonlinearity with respect to the linear component $\Omega^2 >> 4\chi(X^2)$,

$$\frac{\partial^2 X}{\partial t^2} + \gamma\frac{\partial X}{\partial t} + [\Omega^2]X = \frac{\alpha' E_p^*(0)E_s(0)}{M}\exp[i\Omega_0 t] \qquad (23)$$

The solution to this equation is the solution to the homogeneous equation $\frac{\partial^2 X}{\partial t^2} + \gamma\frac{\partial X}{\partial t} + \Omega^2 X = 0$ plus a solution to the inhomogeneous equation $X = \exp[\lambda t]$. We find solutions of the homogeneous equation in the form: $\lambda^2 + \gamma\lambda + \Omega^2 = 0$, where

$$\lambda = -\frac{\gamma}{2} \pm i\sqrt{-\frac{\gamma^2}{4} + \Omega^2} = -\frac{\gamma}{2} \pm i\Omega\sqrt{1 - \frac{\gamma^2}{4\Omega^2}};$$

$$X = C\{\exp[\{-\frac{\gamma}{2} + i\Omega\}t] + \exp[\{-\frac{\gamma}{2} - i\Omega\}t] = 2C\exp[\{-\frac{\gamma}{2}t\}\{\frac{\exp[i\Omega t] + \exp[-i\Omega t]}{2}\} = 2C\exp[\{-\frac{\gamma}{2}t\}\cos(\Omega t);$$

$$\exp[i\Omega t] = \cos(\Omega t) + i\sin(\Omega t);$$

$$\exp[-i\Omega t] = \cos(\Omega t) - i\sin(\Omega t);$$

The solution to the homogeneous equation attenuates and it makes no sense to calculate it: $X(t) = X_0 \exp[i\Omega_0 t]$,

$$\frac{\partial^2 X}{\partial t^2} + \gamma \frac{\partial X}{\partial t} + [\Omega^2]X = A(0)\exp[i\Omega_0 t] \cdot$$

If the light is continuous then: $\frac{\alpha' E_p^*(0)E_s(0)}{M}\exp[i\Omega_0 t] = A(0)\exp[i\Omega_0 t]$, it results that $A(0) = \frac{\alpha' E_p^*(0)E_s(0)}{M}$.

But if the light is pulsed then $\frac{\alpha' E_p^*(t)E_s(t)}{M}\exp[i\Omega_0 t] = A(t)\exp[i\Omega_0 t]$; The derivative of A(t) is much smaller than $\Omega_0 |A(t)|$, and in such a situation $|\Delta A(t)/\Delta t| << \Omega_0 |A(t)|$. From the differential equation, the following expression results for the amplitude of the laser pulse at the output.

$$(i\Omega_0)^2 X_0 \exp[i\Omega_0 t] + \gamma i\Omega_0 X_0 \exp[i\Omega_0 t] + \Omega^2 X_0 \exp[i\Omega_0 t] = A(0)\exp[i\Omega_0 t] \rightarrow \quad (24)$$

$$X_0\{\Omega^2 - \Omega_0^2 + i\gamma\Omega_0\} = A(0) \rightarrow X_0 = \frac{A(0)}{\Omega^2 - \Omega_0^2 + i\gamma\Omega_0} \ . \quad (25)$$

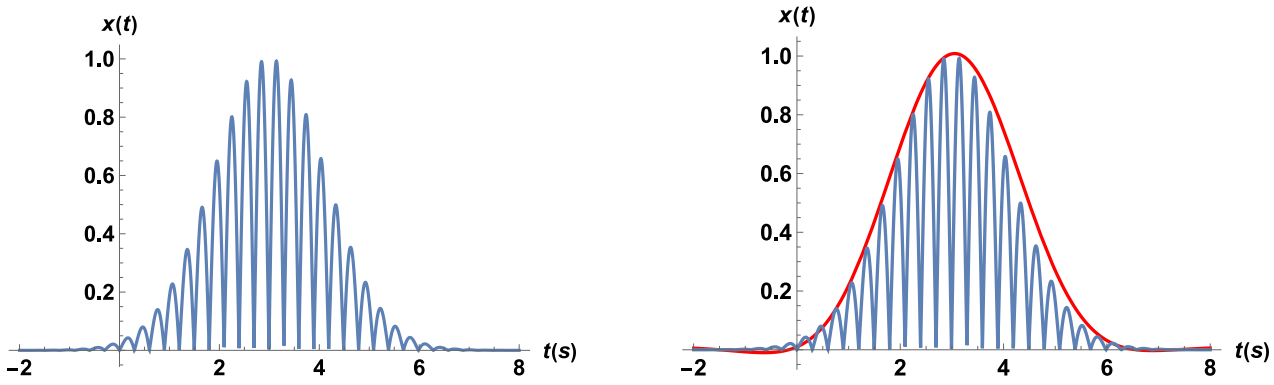
This solution must be introduced into the linear equation for the oscillator (2.8) when renormalizing the frequency: $\Omega^2 - 4\chi X^2$ is replaced with $\Omega^2 - 4\chi X_0^2$, so that the frequency of the new oscillator becomes non-normalized $\tilde{\Omega}^2 = \Omega^2 - 4\chi X_0^2$. The calculation procedure starts again in equation (24). Of course, we will get a $\bar{X}$ which is expressed by the unnormalized oscillator frequency, similar to the solution (2.15). After finding the new solution we return to the oscillator again and instead of X_0^2 we introduce $\bar{X}_0^2$. What we observe is that the amplitude will start to increase when there is a deviation from the resonance. $\Delta^2 = \tilde{\Omega}^2 - \Omega_0^2$ is positive, then the renormalization leads to reaching the parameter value $\Delta^2 = \Omega^2 - \Omega_0^2 - 4\chi X_0^2$ tends to zero and the excitation of the molecules occurs in an avalanche. This leads to an effective dimerization. Let's investigate case 2 when the pulse duration is much smaller than the frequency.

$X_0 \exp[i\Omega_0 t]C;$ $\quad |\Delta A(t)/\Delta t| >> \Omega_0 |A(t)|$, $\frac{\partial^2 X}{\partial t^2} + \gamma \frac{\partial X}{\partial t} + \Omega^2 X = A(t)$ where,

$A(t) = \frac{\alpha' E_p^*(m)E_s(m)}{M}\exp[-(t-t_0)^2/2\tau_p^2]$, τ_p - pulse duration or its width in time $\tau_p << \Omega_0^{-1}$.

It is known from the literature that during laser emission the light is not completely monochromatic. Due to the fact that the excited molecules move thermally, some of them enter into resonance with the generation line, and some leave this generation

frequency. Because the planar resonator has multiple frequencies $2\pi C/\lambda$ The resonator in the resonance line of the molecules at UV-C emission hits a lot of these frequencies as shown in Fig. 5.b.



a) **b)**

Fig. 5. a) Graphical representation of the oscillation frequency of the molecules b) The envelope or pulse shape in relation to the oscillation frequency of the molecules given by the expression $\exp[-(t-t_0)^2/\tau^2]\sin(\omega t)$ **with values**

$$\tau = 1.6; t_0 = 3; \omega = 20$$

The distance between these natural frequencies of the resonator is equal to $2\pi C/\lambda$, so this frequency can be of the order of terahertz, the frequency often encountered in bimolecular vibrations. When multiplying the electric field intensity of the same pulse $E \times E$ there will certainly be combinations of such frequencies at the differences. These differences at the exponent can cause vibrations of the order of terahertz. Namely on the right side of the oscillator equation such frequencies are encountered and not at all the laser frequency in UV-C. Here a resonance between the difference in frequencies for E and E^*, and the frequency of the molecular vibrations described above. We studied this in the first case and demonstrated the resonance transition effect upon nonlinear excitation of biomolecules. However, in certain circumstances this heavy resonance effect can be omitted. For example, when the pulse duration is shorter than the vibration period, the pulse intensity and not its frequency come into play. In this case we can solve the problem using Green's functions and also remove the frequency dependence in front of the integral in the solution:

$$Z(t) = C_0 \exp[(i\Omega - \gamma/2)t] + \int_0^\infty dt' A(t')\theta(t-t')\exp[(i\Omega - \gamma/2)(t-t')].$$

Chapter three, *"The influence of UV-C radiation intensity on the rate of pathogen decontamination"*, analyzes the application of the Born-Oppenheimer (B-O) approximation in the context of UV-C radiation-induced DNA dimerization, a key process in modifying the molecular structure of DNA. The B-O approximation is based on the separation of the motion of atomic nuclei from that of electrons, due to the significant difference in mass and speed between them, electrons being much faster and lighter. This separation allows the modeling of molecular dynamics in a simplified way, treating the nuclei as quasi-static during the motion of electrons.

The idea of this approximation is based on the assumption that the wave functions of atomic nuclei and electrons in a molecule can be treated separately, based on the fact that nuclei are much heavier than electrons. Since the relative mass of a nucleus is larger compared to the mass of an electron, the B-O approximation assumes that the nuclei can be fixed at the time intervals for which the electronic subsystem passes into a quantum state determined by the interactions between electrons [16]. To describe the dimerization process, a nonlinear model of the interaction between the molecular subsystems of DNA and laser pulses is proposed. It is assumed that, as these subsystems are excited, the vibrational frequency decreases proportionally to the excitation amplitude. In this context, a dimerization algorithm based on the renormalization of the vibrational frequency after each pulse is proposed, allowing a dynamic description of the process.

Starting from the B-O approximation below, we consider the molecular energy as a sum of terms containing the following interactions:

$$\hat{H} = \sum_{\alpha=1}^{N_n} \{ \frac{\hat{P}_\alpha^2}{2M_\alpha} + V(r, R_\alpha) \} + \sum_{k=1}^{N_e} \frac{\mathbf{p}_k^2}{2m}, \tag{26}$$

where, P_α , $\mathbf{R}_\alpha$, M_α, si $\mathbf{p}_k$, $\mathbf{r}_k$, m are the impulses, the positions of the masses of N_n nuclei and N_e valence electrons, respectively; $V(r,R)$ is the Columbian energy of the interaction between electrons and nuclei described by the expression which can be represented as the sum of 3 terms : $V(r,R) = V_N(R) + V_E(\mathrm{r}) + V_{N,E}(r-R)$, where $V_N(R) = \sum_{\alpha,\beta=1}^{2} \{ \sum_{j<k} U(|\mathbf{R}_{j\alpha} - \mathbf{R}_{k\beta}|)$ contains the electromagnetic and exchange interaction between nuclei; $V_E(r) = \sum_{j<k} \frac{e^2}{|\mathbf{r}_j - \mathbf{r}_k|}$ is the Columbian interaction between electrons. The last term contains the interaction between the fast electron subsystem and the nuclei subsystem

$V_{N,E}(r-R)=\sum_{\alpha,\beta=1}^{2}\sum_{j<k}\frac{e_j e_k}{|\mathbf{R}_{j\alpha}-\mathbf{r}_{k\beta}|}$. Here e_j and e_k are the electrical charges of the nucleus j and of that electron; R_j and r_k are electron position vectors k and the nucleus j. Let us first study the nonlinear vibration of the lattice. In the adiabatic approximation we can introduce the displacement $\xi_{j\alpha}=R_{j\alpha}-R^0_{j\alpha}$. In this case we can consider the potential energy $U(R)\simeq\sum_{j<k}\frac{e_j e_k}{\left|R_j-R_k\right|}$ in the Taylor series relative to its equilibrium state up to order 4 after the small parameter $\xi_{j\alpha}/R^0_{j\alpha}$.

$$U(R)=U(R_0)+\frac{1}{2}\sum_{\alpha=1}^{3}\sum_{l,j}\frac{\partial^2 U}{\partial R_{l\alpha}\partial R_{j\alpha}}\xi_{j\alpha}\xi_{l\alpha}+\sum_{\alpha<\beta}^{3}\sum_{l,j}\frac{\partial^2 U}{\partial R_{l\alpha}\partial R_{j\beta}}\xi_{j\alpha}\xi_{l\beta}$$
$$+\frac{1}{4!}\sum_{l,j,m,n}\frac{\partial^4 U}{\partial R_l\partial R_j\partial R_m\partial R_n}\xi_j\xi_l\xi_m\xi_m.$$

According to [16] in a vibration of nonlinear lactics in one dimension, this Hamiltonian is reduced to the simplest form

$$\hat{H}'_v=\sum_{j=1}^{N}\frac{\hat{\mathbf{P}}_j^2}{2M}+K\sum_{j}^{N}\frac{(\xi_j-\xi_{j-1})^2}{2}+A\sum_{j=1}^{N}(\xi_j-\xi_{j-1})^4,$$

where K and A are the harmonic and enharmonic coefficients in the direction ξ_j.

As a method for analyzing molecular systems in quantum mechanics, the B-O approximation is a variation of the adiabatic approximation of the Schrödinger equation, which consists in identifying and describing separately the atomic nuclei and the electrons in the system, for which the characteristic times of state change are very different. In the language of quantum mechanics, the B-O approximation is equivalent to the assumption that the total wave function Ψ_t of a molecule can be expressed as the product of an electronic wave function Ψ_e and of a nuclear wave function Ψ_n (vibrational, rotational):

$$\Psi_t(r,R)=\Psi_e(r,R)\times\Psi_n(R), \tag{27}$$

where $r-$ are the electron coordinates, and $R-$ are the coordinates of the nuclei.

The non-stationary Schrödinger equation for a molecule with n nuclei and n electrons and an approximating wave function takes the form:

$$\left(\sum_{\alpha=1}^{N} \frac{[\hat{P}\alpha + \frac{e_\alpha}{c} A(R_\alpha,t)]^2}{2M_\alpha} + \sum_{i=1}^{n} \frac{[\hat{p}_i - \frac{e_\alpha}{c} A(r_i,t)]^2}{2m_e} + V(r,R) + U(r,R) \right) \times$$

$$\times \Psi_e(r,R,t) \times \Psi_n(R,t) = i\hbar \frac{\partial}{\partial t} \Psi_e(r,R,t) \times \Psi_n(R,t), \quad (28)$$

where, $A(R_\alpha,t)$ and $A(r_i,t)$ is the vector potential of the electromagnetic field applied to the molecular system, respectively for nuclei and electrons. $U(r,R)$ describes the interaction of the molecular system with the scalar component of the electromagnetic field applied to the system of electrons and nuclei. From the calibration of the electromagnetic field one can choose the case when the scalar part becomes negligible compared to the vector part of the field for transverse electromagnetic waves. The interaction of charges with electromagnetic waves can be calculated using the time-dependent perturbation theory. In the calibration of radiation when $\vec{\nabla} \cdot \vec{A} = 0$, we can decompose the square of the displaced momenta in the Schrödinger equation (26) in series. For example, for nuclei we obtain the following addition to $P^2/2M$

$$V_{ph}^{n} = \frac{e_\alpha}{Mc} \vec{A}(R,t) \cdot \vec{P} + \frac{e_\alpha^2}{2Mc^2} A^2(R,t); \quad V_{ph}^{e} = -\frac{e}{mc} \vec{A}(r,t) \cdot \vec{p} + \frac{e^2}{2mc^2} A^2(r,t).$$

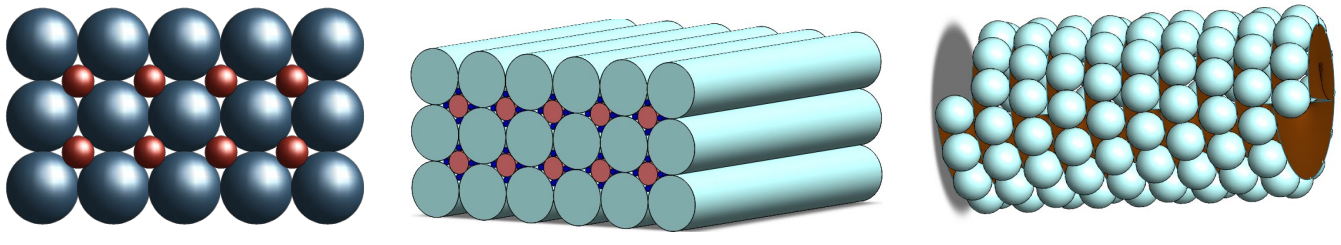
We note that the interaction potential with the electromagnetic field can be taken in the non-relativistic approximation by neglecting the last terms in both expressions above proportional to A^2. We also note that the first term on the electronic side can be larger than the interaction potential of the nuclei with the electromagnetic field. This occurs because the mass of the electron, m, is much smaller than the mass of the nuclei M. We also consider that in the radial direction of electronic transitions towards nuclei, the law of conservation of momentum of electrons and nuclei in interaction takes place P proportional to p. This assumption allows us to completely neglect the interaction of nuclei with the electromagnetic field, considering only the potential for electrons in the non-relativistic approximation. $V_{ph}^{e} = -\frac{e}{mc} \vec{A}(r,t) \cdot \vec{p}$. For most atomic decays, the term A^2 can be neglected because it is much smaller than the product $\vec{A} \cdot \vec{p}$. It is possible to calculate both the decay of excited atomic states with the emission of radiation and the excitation of atoms with the absorption of radiation. An arbitrary electromagnetic field can be analyzed using Fourier decomposition to give a sum of components of defined frequency. If we consider the vector potential for such a

component, $\vec{A}(\vec{r},t) \equiv 2\vec{A}_0 \cos(\vec{k}\cdot\vec{r}-\omega t)$. The energy in the field is $E = \frac{\omega^2}{2\pi c^2} V |A_0|^2$. If the field is quantized with energy photons $E = \hbar\omega$, we can write the field intensity in terms of N photons.

$$\vec{A}(\vec{r},t) = \left[\frac{2\pi\hbar c^2 N}{\omega V}\right]^{\frac{1}{2}} \hat{\varepsilon}\cos(\vec{k}\cdot\vec{r}-\omega t). \tag{29}$$

The direction of the field is given by the unit polarization vector. The cosine term has been divided into positive and negative exponentials. In time-dependent perturbation theory, the positive exponential corresponds to the absorption of a photon and the excitation of the atom, and the negative exponential corresponds to the emission of a photon and the decay of the atom to a lower energy state.

Chapter Four, *"Application of Rotational Channels for Pathogen Decontamination in Metamaterials Penetrated by UV-C Radiation,"* explores the use of metamaterials exposed to UV-C radiation for pathogen decontamination, focusing on the manipulation of biomolecules through rotational channels and evanescent optical fields. The interaction of pathogens with metamaterials under the influence of UV-C radiation was analyzed, highlighting the mechanisms of biomolecule capture and manipulation in evanescent optical fields. It was demonstrated that composite metamaterials, configured in spherical and cylindrical geometries, significantly enhance the decontamination rate of infected solutions due to the amplification of photonic interactions [17,18]. To improve the contact surface between pathogens and UV-C radiation, a combination of metamaterial elements, such as spheres and fibers, was used in packing arrangements [19]. In this way, larger elements allow UV-C radiation to travel a greater distance within contaminated liquids, while smaller elements filling the free space between them ensure optimal radiation dispersion in large volumes (Fig. 6).



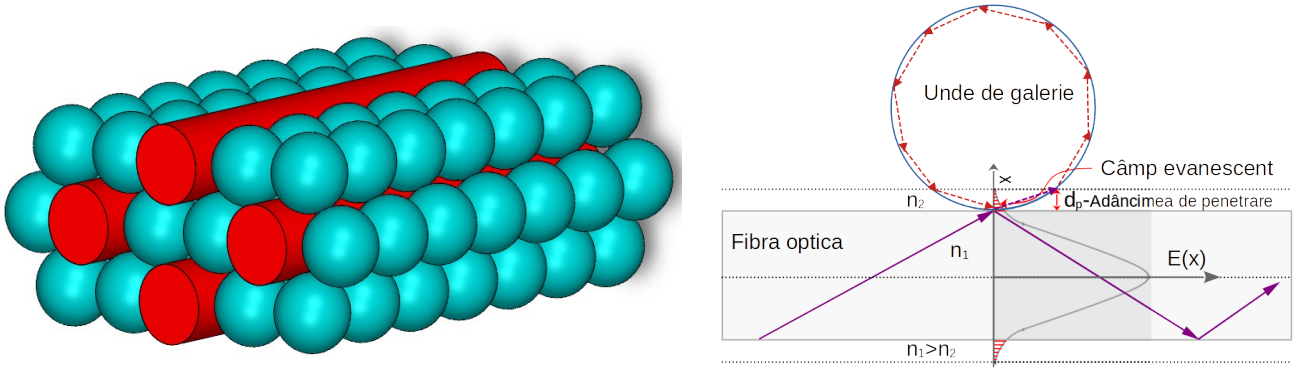
a) **b)** **c)**

Fig.6 a) Packing of small/large balls (a), respectively fibers (b), screw channels.

The free space between large quartz spheres can be described by a filling factor, which is a function of the metamaterial packing structure, $V_f = V(1-\rho),$ where V_f is the free volume between the spheres, is the total volume and the density of the cell, which depends on the packing structure of the metamaterial. In the case of hexagonally arranged quartz balls Fig. 6.b the density is $\rho = \pi / (3\sqrt{3}) = 0,6086,$ which is superior to the tetrahedral lattice packing Fig. 4.2a, for which $\rho = (\pi\sqrt{3})/16 = 0,3401.$ This means that the free volume in the tetragonal packing is larger than in the hexagonal one.

It is generally accepted that the penetration depth, k inside the free space between the spheres is directly proportional to the wavelength of the radiation and inversely proportional to the difference between the refractive indices of the metamaterial, n_m and contaminated fluid n_f, in that case $k = \lambda / \left[2\pi\sqrt{(n_m^2 - n_f^2)}\right].$ It follows that the effective volume is $V_u = kS$ where S represents the contact surface of the metamaterial with the contaminated fluid. This volume is kept lower than the free volume between the spheres, V_f. The relationship between the diameter of the sphere D, and the total surface area of the spheres can be written as: $S = pD^2N,$ where N represents the total number of spheres. If we consider L_i, where $i = (x, y, z)$ a direction in space, volume $V = L_x L_y L_z$ is completed with, $N_i = L_i/D$ which is the number of spheres in each direction, accumulating a total of spheres in his cell where the number $N = N_x N_y N_z.$ This number is proportional to the volume: $N \sim V/D^3$. The effective volume of decontamination around the packed spheres is proportional to the penetration depth, $\kappa \sim \lambda$ and inversely proportional to the diameter of the sphere, $V_u \sim V\lambda/D.$ In the case of small diameter spheres $V_{fi} = V(1-\rho)^{(i-1)},$ in the case of smaller diameter spheres D_{i-1}.

A packing model of the beads combined with quartz rods/fibers, shown in figure 7 where the total surface area of these metamaterials in contact with the contaminated fluids is in this case significantly increased, with beneficial effects on decontamination because the radiation is dispersed by evanescent waves in an extended volume of circulating fluids. This type of packing of the rods in combination with the fibers makes it possible for the radiation dispersion to persist both longitudinally and transversely, and thus the free areas between the beads/fibers to be equally penetrated by the radiation.



a) **b)**

Fig. 7. a) Arrangement of balls combined with quartz rods; b) Gallery waves occurring at the contact between the fiber and the ball

Due to the evanescent zone forming around the entire surface of the fibers [20], which penetrates the sphere upon contact, creating so-called whispering gallery modes (Fig. 7b) that are highly significant in the pathogen decontamination process. Furthermore, the evanescent zone covers a substantial portion of the sphere's surface. If we compare this sphere to pathogens with diameters more than ten times larger than the penetration depth of the evanescent wave, the resulting whispering gallery modes can induce negative effects, rendering the cell incapable of reproduction.

When light interacts with a quartz sphere immersed in a yeast solution, at a wavelength of $254nm$, an evanescent zone forms at the interface between the two media. The depth of this zone depends on the angle of incidence of the light and the refractive indices of the materials involved.

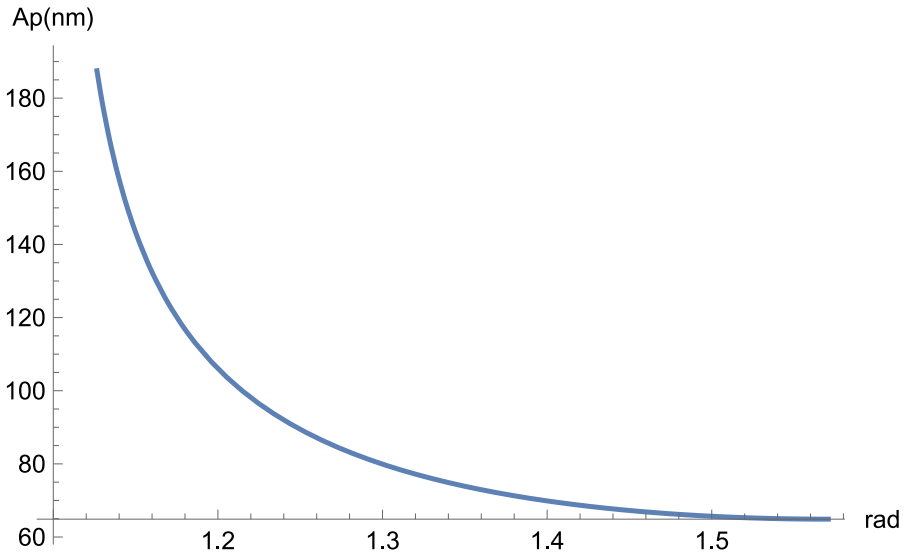


Fig. 8. Dependence of the penetration depth of electromagnetic radiation in the environment n_2 (yeast solution) from the environment n_1 (quartz ball) by the angle of incidence. Simulation performed in Wolfram Mathematica

To calculate the depth of the evanescence zone for a quartz sphere in yeast solution, with a wavelength of $256\,nm$ and an angle of incidence of $\theta = 65{,}89^{\circ}$, (randomly chosen from the graph in Fig.8) so that the condition for total internal reflection is met, the standard formula for the penetration depth will be used A_p of the evanescent field: $A_p = \frac{\lambda}{2\pi} \cdot \frac{1}{\sqrt{n_1^2 \sin^2\theta - n_2^2}}$. The thickness of the evanescence zone is $\delta = A_p \approx 115.83\,nm.$ Here, we proposed as a goal to calculate the remaining volume in a cube of side $1\,cm$, where is it located $N = 1000$ of quartz balls, each having $1\,mm$ diameter, including the evanescent layer. We will then exclude the total volume occupied by these balls along with their evanescent areas to see the remaining volume which is nothing more than the volume of the yeast solution: $S_{evanescent(R)} = 4\pi R^2 = 3.14 mm^2$. We apply the volume formula for a thin spherical layer which is nothing more than the difference between two spheres: $V = \frac{4}{3}\pi[(R + A_p)^3 - R^3]$. For $A_p \ll R$, we can approximate with $V_{evanescent} \approx 4\pi R^2 \cdot A_p \approx S_{evanescent(R)} \cdot A_p$, which is a first-order approximation, suitable for very thin areas, takes the value: $V_{evanescent} \approx 0.0003638\,mm^3$; **The volume of a ball of radius R will be equal to:** $V_B = \frac{3}{4}\pi R^3 = 5.24 \times 10^{-10} m^3$; The total volume occupied by the balls, plus the volume of the evanescent zones, is: $V_{total} = 1000 \cdot (V_B + V_{evanescent}) = 5.24 \times 10^{-7} m^3.$ The remaining volume of the cube is nothing more than the volume occupied by the yeast, so: $V_{drojdie} = V_{cub} - V_{total} = 0.476 mm^3.$

The volume of the evanescence zone and the remaining free volume in a cube with a side of 10 mm, in which balls of diameter 1 mm are placed, and in the free spaces between them smaller balls of diameter are inserted $d = \sqrt{2} - 1\,mm$, and the number of **interior unit cubes** (excluding the exterior edges) is $(10-1)^3 = 729$ **holes** into which balls can be inserted. **The surface area of a ball of radius** $r = \frac{d}{2} = \frac{\sqrt{2}-1}{2} \approx 0.207 mm$ **is:** $S_{evanescent(r)} = 4\pi r^2 = 0.5372\,mm^2.$

The volume of the evanescence zone for 729 balls of radius r **will be equal to:**

$$V_{evanescent(r)} = N \times S_{evanescent(r)} \times A_p \approx 0.0000622 mm^3.$$

The total volume of the vanishing zone created around the radius balls $R + r$ **is:**

$$V_{evanescenta(R+r)} \approx 0.3638 + 0.0453 = 0.4091 mm^3.$$

GENERAL CONCLUSIONS AND RECOMMENDATIONS

This thesis addresses two major research directions: the first focuses on the interaction of short pulses with biomolecules, while the second investigates the use of the evanescent zone generated by introducing transparent metamaterials into translucent fluids.

The DNA of microorganisms is affected by photons in the UV-C spectrum (200–280 nm), which induce thymine dimers and other structural changes leading to their inactivation. The Born–Oppenheimer (B-O) model, applied to the interaction of biomolecules with UV-C radiation, enables the modeling of molecular-level structural changes caused by photonic absorption and the formation of thymine dimers in pathogen DNA. The B-O approximation can be used to predict the probability of microorganism inactivation based on the wavelength, intensity, and duration of exposure to pulsed UV-C radiation. Since interactions between ultraviolet radiation and DNA involve both electronic transitions (excitation of electrons in DNA molecules) and slow nuclear processes (structural deformations of the macromolecule), the B-O approximation allows these processes to be treated separately. These theories were developed by applying the B-O model to DNA dimerization under UV-C radiation. To increase the inactivation rate of pathogens in infected solutions, the use of translucent quartz metamaterials was proposed, which enhance light penetration, thereby increasing the evanescent field around each metamaterial element and significantly reducing the exposure time required.

Recommendations: UV-C radiation is used in sterilization and decontamination due to its germicidal properties, but it also poses significant risks to human health and the environment. For this reason, its use must be regulated by international and national standards to avoid negative impacts on public health and the environment.

Human exposure should be avoided, as UV-C radiation can cause eye injuries, skin burns, and cellular DNA damage, increasing the risk of skin cancer. UV-C systems must be used in controlled environments, with decontamination performed in the absence of personnel or using protective shields and safety sensors that halt emission upon detecting human movement. UV-C equipment must comply with international standards regarding wavelength, radiation dose, and user safety.

BIBLIOGRAPHICAL REFERENCES

1. KOWALSKI, W. UVGI disinfection Theory. În: Ultraviolet germicidal irradiation handbook, *Springer*, 2009, pp.17-50.
2. ENAKI, N.A., **MUNTEANU, I.,** PASLARI, T., TURCAN, M., STARODUB, E., BAZGAN, S., PODOLEANU, D., RISTOSCU, C., ANGHEL, S., BADICEANU, M., Anghel, S., Badiceanu, M., Mihailescu, I.N. Topological Avenue for Efficient Decontamination of Large Volumes of Fluids via UVC Irradiation of Packed Metamaterials. În: *Materials.* 2023, vol. 16, pp. 45-59.
3. MARA, Biasin et al. UV-C irradiation is highly effective in inactivating SARS-CoV-2 replication. În: Sci Rep 2021, vol 11, pp. 62-60. doi.org/10.1038/s41598-021-85425-w
4. BUONANNO, M., WELCH, D., SHURYAK, I. *et al.* Far-UVC light (222 nm) efficiently and safely inactivates airborne human coronaviruses. În: Sci Rep, 2020, vol. 10. doi.org/10.1038/s41598-020-67211-2
5. LYTLE CD, SAGRIPANTI JL. Predicted inactivation of viruses of relevance to biodefense by solar radiation. În: J Virol. 2005, vol. 79. doi: 10.1128/JVI.79.22.14244-14252.2005
6. ZHANG, C., LI, Y., SHUAI, D., SHEN, Y., WANG, D. Progress and challenges in photocatalytic disinfection of waterborne viruses: a review to fill current knowledge gaps. În: *Chem. Eng. J*. 2019 vol. 355, pp. 399–415.
7. **MUNTEANU, I.,** STARODUB, E., BAZGAN, S., TURCAN, M., PASLARI, T., PODOLEANU, D., ENAKI, N.A. Ultraviolet C intensity dependence of decontamination efficiency for pathogens as function of repacked metamaterials with screw channels. În: *Eur Biophys J*. 2024, vol. **53(3)**, pp. 133—145. doi. 10.1007/s00249-024-01702-2
8. YARIV, A. Critical coupling and its control in optical waveguide-ring resonator systems. În: *IEEE Photon. Technol. Lett.* vol. 14, pp. 483–485
9. YARIV, A.: Universal relations for coupling of optical power between microresonators and dielectric waveguides. În: *Electron. Lett.* vol. 36, pp. 321–322
10. GORODETSKY, M. L., and ILCHENKO, V. S. Optical microsphere resonators: optimal coupling to high-Q whispering-gallery modes. În: *Journal of the Optical Society of America B.* 1999, vol. 16(1), p. 147. doi:10.1364/josab.16.000147
11. HANSON, DAVID. "The Born-Oppenheimer Approximation". Chemistry Libretexts. În: *Chemical Education Digital Library.* Retrieved 2

August 2022.
12. BORAAS, M.E.; SEALE, D.B.; BOXHORN, J.E. Phagotrophy by a flagellate selects for colonial prey: A possible origin of multicellularity. În: Evol. Ecology (1998). Vol 12, p. 153 https://doi.org/10.1023/A:1006527528063
13. BORN, M., OPPENHEIMER, J. R. Zur Quantentheorie der Molekeln [On the Quantum Theory of Molecules]. În: Annalen der Physik (in German). 1927 vol. 389(20), p. 457–461.
14. SCHUBERT, M., WILHELMI, B. Nonlinear Optics and Quantum Electronics. În: *Wiley*. 1986, 752 p., ISBN 0471088072, 9780471088073
15. SHEN, Y.R., BLOEMBERGEN, N. Theory of simulated Brillouin and Raman scattering. În: *Phys Rev,* 1965, vol. 137.
16. ENAKI, N.A., PROFIR, A., CIOBANU, N., BAZGAN, S., NISTREANU, A., TURCAN, M., STARODUB, E., PASLARI, T., RISTOSCU, C., BADICEANU, M., MIHAILESCU, I.N. Optical metamaterials for decon-tamination of translucent liquids and gases, În: *J Phys D.* 2018, vol. 51, pp.385101-11.
17. PEREPECHKIN, L.P., PEREPECHKINA, N.P. Chemistry and technology of chemical fibres hollow fibres for medical applications. a review a few words on mass transfer processes in the body. În: *Fibre Chem*. 1999, vol. 31, pp. 411–420
18. PASLARI, T., STARODUB, E., TURCAN, M., **MUNTEANU, I.,** BAZGAN, S., ENAKI, N.A. Improvement of ultraviolet C decontamination rate using composite quartz metamaterial. În: *GSC Bio Pharm Sciences*. 2022, vol. 20(3), pp. 187—191. doi.10.30574/gscbps.2022.20.3.0263.
19. **MUNTEANU, I.,** TURCAN, M., STARODUB, E., BAZGAN, S., NISTREANU, A., PASLARI, T., ENAKI. N.A. Ultraviolet C Radiation for Disinfection and Protection Using Periodical Optical Structure for Dental Implant. În: *IEEE Xplore, E-Health and Bioengineering Conference (EHB),* 17-18 November 2022, Iasi, Romania p. 1—4. Doi: 10.1109/EHB55594.2022.9991449
20. SKELTON, S.E., SERGIDES, M., PATEL, R., KARCZEWSKA, E., MARAGÓ, O.M., JONES, P.H. Evanescent wave optical trapping and transport of micro- and nanoparticles on tapered optical fibers. În: *Journal of Quantitative Spectroscopy and Radiative Transfer*. 2012, vol. 113, issue 18, pp. 2512-2520.

LIST OF THE AUTHOR'S PUBLICATIONS ON THE THESIS TOPIC

Journal articles from the Web of Science and SCOPUS databases

1. ENAKI, N.A., PASLARI, T., BAZGAN, S., STARODUB, E., **MUNTEANU, I.,** TURCAN, M., EREMEEV, V., PROFIR, A., MIHAILESCU, I.N. UVC radiation intensity dependence of pathogen decontamination rate: semiclassical theory and experiment. În: *Eur Phys J Plus*. 2022, **137(9)**, 1047-1—1047-14. Doi: 10.1140/epjp/s13360-022-03252-y (IF: 2,7).

2. ENAKI, N.A., **MUNTEANU, I.,** PASLARI, T., TURCAN, M., STARODUB, E., BAZGAN, S., PODOLEANU, D., RISTOSCU, C., ANGHEL, S., BADICEANU, M.; MIHAILESCU, I.N. Topological avenue for efficient decontamination of large volumes of fluids via UVC irradiation of packed metamaterials. În: *Materials*. 2023, **16(13)**, 4559-1—4559-13. Doi: 10.3390/ma16134559. (IF 3,4).

3. MUNTEANU, I., STARODUB, E., BAZGAN, S., TURCAN, M., PASLARI, T., PODOLEANU, D., ENAKI, N.A. Ultraviolet C intensity dependence of decontamination efficiency for pathogens as function of repacked metamaterials with screw channels. În: *Eur Biophys J*. 2024, **53(3)**, 133—145. Doi: 10.1007/s00249-024-01702-2 (IF: 2,2).

Articles in journals from other databases accepted by ANACEC

1. MUNTEANU, I. Action Of UV-C Radiation for Biomolecules Inactivation, With Application in Diagnostics. În: *Biomed J Sci & Tech Res*. 2023, **52(1)**, 43282—43287. Doi: 10.26717/BJSTR.2023.52.008192

2. STARODUB, E., **MUNTEANU, I.,** BAZGAN, S., PODOLEANU, D., COSTISEN, I., ENAKI, N.A. Construction of Rotation Channels for Pathogens Using the Repacking Method of Elements from Metamaterial Penetrated By Ultraviolet C Radiation. În: *Phys Sci & Biophys J*. 2023, **7(2)**, 256-1—256-11. Doi: 10.23880/psbj-16000256.

3. MUNTEANU, I., STARODUB, E., ENAKI, N.A. Influence of Ultraviolet Radiations Against Bacteria, Fungi, Fungal Spores. Determination of UV Action Spectra Affecting the Infection Process. În: *Biomed J Sci & Tech Res*. 2023, **50(2)**, 41448—41454. Doi: 10.26717/BJSTR.2023.50.007920.

4. ENAKI, N.A., MUNTEANU, I., TURCAN, M., BAZGAN, S., PASLARI, T., STARODUB, E. Application of Rotation Channels for Decontamination of Pathogens in Metamaterials Penetrated by UVC Radiation. În: *J Infections Diseases Preventive Medicine*. 2023, **11(2)**, 1000296-1—1000296-3. Doi: 10.35841/2329-8731.23.11.296.

5. PASLARI, T., STARODUB, E., TURCAN, M., **MUNTEANU, I.,** BAZGAN, S., ENAKI, N.A**.** Improvement of ultraviolet C decontamination rate using composite quartz metamaterial. În: *GSC Bio Pharm Sciences*. 2022, **20(3)**, p.187—191. Doi: 10.30574/gscbps.2022.20.3.0263.

Articole în reviste din Registrul Național al revistelor de profil (cu indicarea categoriei)

1. MUNTEANU, I. Mecanism de inactivare a agenților patogeni cu aplicare în implantologie. În: Studia Universitatis Moldaviae, Revista științifică a Universtității de Stat din Moldova, 2024, nr. 1(171), 109-115.CZU: 535.37:616.314-089. (Categoria B)

Doi.org/10.59295/sum1(171)2024_13. Link: https://natural.studiamsu.md/nr-1-171/

Articles in the proceedings of scientific events included in the Web of Science and SCOPUS databases

1. MUNTEANU, I., TURCAN, M., STARODUB, E., BAZGAN, S., NISTREANU, A., PASLARI, T., ENAKI. N.A. Ultraviolet C Radiation for Disinfection and Protection Using Periodical Optical Structure for Dental Implant. În: *IEEE Xplore, 2023*. 2022 E-Health and Bioengineering Conference (EHB), 17-18 November 2022, Iasi, Romania , p. 1—4 . Doi: 10.1109/EHB55594.2022.9991449

2. PODOLEANU, Diana., COSTISEN, Igor., **MUNTEANU, Ion.,** STARODUB, Elena., ENACHI, Nicolae. „*The Generation of Photonic "Molecules" Under the Action of Ultraviolet Light in the DNA/RNA Dimerization Process*" IEEE Conference Advanced Topics on Measurement and Simulation (ATOMS), Constanta. Romania. http://atoms2024.org/program.html

Articles in the proceedings of scientific events included in the Register of materials published in the database of scientific events organized in the Republic of Moldova

1. MUNTEANU, I., STARODUB, Elena. Radiații ultraviolete-c utilizate în dezinfecție și protecția suprafeței implanturilor. In: *Conferința tehnico-științifică a studenților, masteranzilor și doctoranzilor*, 5-7 aprilie 2023, Chișinău. Chișinău, Republica Moldova: Tehnica-UTM, 2023, Vol.2, pp. 158-162. ISBN 978-9975-45-956-3. https://ibn.idsi.md/vizualizare_articol/188467

2. MUNTEANU, I. Procedura de inactivare a patogenilor pentru dezinfecția si protecția suprafeței implantului. Conferința științifico-practică internațională „Instruire prin cercetare pentru o societate prosperă", Ediția a XI-a, 16-17 martie, 2024, Volumul I, Chișinău, Moldova, p. 240—245, CZU: 535:61, Doi: 10.46727/c.v1.16-17-05-2024. Link: https://drive.google.com/file/d/1FVF3LpuwKz6tShC1IUqyBNLFC_KuNZE8/view

3. MUNTEANU, Ion, CIOBANU, Nellu. New methods of pathogen inactivation using uv-c radiation. Conferinta Nationala cu Participare Internationala: ȘTIINȚELE ale NATURII ÎN DIALOGUL GENERAȚILOR, editia VII, 12-13 septembrie 2024, Chișinău, Republica Moldova.

4. MUNTEANU, I. Procedeu de inactivare a agenților patogeni sub acțiunea UVC cu aplicare în implantologie. Conferința științifico-practică „TEHNOLOGII FIZICE AVANSATE CU APLICAREA UVS ÎN MONITORIZAREA ȘI MODELAREA FACTORILOR DE MEDIU", Ediția a V – a, 8 Noiembrie 2024, Chișinău, [Editura USM], p. 55-62, CZU: 535.37:615.371:616.314-77

Patents and other intellectual property (IP)

1. MUNTEANU, I., ENACHI, N. Device for decontamination of liquids. Patent no. MD 1723 Y 2023.10.31.

2. MUNTEANU, I., ȚURCAN, M. Sterilizing device. Short-term patent MD s 2024 0049 granted based on decision no. 225 of 10.01.2025

3. MUNTEANU, I., UV-C sterilizer device, Short-term patent granted based on decision no. 4057 of 27.03.2025, deposit no.: s 2025 0015

ADNOTARE

la teza „Acțiunea cooperativ cuantica a impulsurilor scurte de radiație cu biomoleculele la propagarea lor prin metamateriale cu aplicarea ei în diagnostica, tratament și inactivarea patogenilor”, prezentată de Munteanu Ion pentru conferirea gradului de doctor în științe fizice la specialitatea 131.01 „ Fizică matematică”.

Structura tezei: Teza a fost perfectată la Institutul de Fizică Aplicată, Universitatea de Stat din Moldova, Chișinău, 2025, scrisă în limba română ce constă din introducere, patru capitole, concluzii generale și recomandări, 135 titluri bibliografice, 122 pagini de text de bază, 46 figuri. Rezultatele prezentate în teză au fost publicate în 15 lucrări științifice. In baza teoriilor dezvoltate am obținut două brevete de invenție, iar altul este in proces de obținere.

Cuvinte-cheie: radiații UV-C pulsate, metamateriale, decontaminare, dimerizare ADN, inactivare patogeni.

Domeniul de cercetare: biofizica, optică neliniară și optica cuantică.

Scopul lucrării: Scopul tezei este de a prezenta rezultatele cercetării referitor acțiunii cooperativ cuantice a impulsurilor scurte de radiație UV-C la propagarea lor prin metamateriale pentru inactivarea agenților patogeni.

Obiectivele cercetării: analiza interacțiunii dintre radiațiile UV-C cu materia; inactivarea agenților patogeni datorita radiației coerente UV-C pulsate aplicate; se propune descrierea neliniară a dependenței ratei de dimerizare ADN/ARN în funcție de radiația ultravioletă C sub forma de pulsuri scurte aplicată; aplicarea modelului Born-Oppenheimer la dimerizarea ADN-lui sub acțiunea radiației; manipularea biomoleculelor cu ajutorul canalelor de rotație prin metamaterialele pătrunse de radiații UVC; posibilitatea aplicării acestor concepții se propune echipamente de decontaminare cu dispersie a radiației în volum prin fibra/meta material sferic în dezinfectarea fluidelor (aer, apa, ser sangvin etc...); se studiază posibilitățile de aplicare și optimizare a intensității radiațiilor UVC aplicate în echipamentul de decontaminare propus pe volumul bazelor metamaterialelor.

Noutatea științifică și originalitatea rezultatelor obținute. Pentru prima dată s-a propus canalizarea radiației UV-C prin diferite sisteme optice speciale (metamateriale) utilizând diferite tipuri de combinări fibre-bile din cuarț. În investigațiile realizate experimental a fost determinat adâncimea de penetrare a radiației UV-C prin astfel de împachetări ale metamaterialelor la diferite intensități, cat si dependenta dozei de radiație în raport cu rata de inactivare a soluției de drojdie. A fost dezvoltat și brevetat un dispozitiv pentru decontaminarea lichidelor și sterilizator UV-C.

Problema științifică importantă soluționată consta în evidențierea unui mecanism de inactivare eficienta in baza cercetărilor teoretice si experimentale luând in considerație corelația lor.

Semnificația teoretică a tezei în constă în dezvoltarea teoriei in modelul (aproximarea) Born-Oppenheimer si aplicarea lui la dimerizarea ADN-lui sub acțiunea radiației ultraviolete de tip C inclusiv dezvoltarea tehnologiilor de decontaminare a agenților patogeni la utilizarea pulsurilor scurte de radiație propagate prin metamateriale pentru creșterea ratei de decontaminare a soluțiilor infectate. Deoarece subsistemul electronic este mai rapid in comparație cu subsistemul de nuclee al biomoleculelor este cercetată soluționarea problemei cuantice de excitare a subsistemului electronic, considerând ca subsistemul atomic de nuclee este lent si poate fi considerat fixat.

Valoarea aplicativă a tezei. Aceasta presupune posibilitatea aplicării rezultatelor cercetării descrise în teză pentru dezvoltarea si elaborarea unor dispozitive de decontaminare cu o rata înalta de inactivare a agenților patogeni, prezenți in medii diferite precum: apa aer si suprafețe.

Implementarea rezultatelor științifice. Rezultatele obținute au fost utilizate în cadrul proiectului instituțional din cadrul Programului de Stat (2020-2023) Proiectul ANCD 20.80009.5007.01: Cooperativitate cuantică între emițători (nuclee, atomi, puncte cuantice, molecule, biomolecule, meta materiale) și aplicarea acesteia în informatică, biofotonică avansată optogenetică, cat si din cadrul subprogramului 011206: Fenomene cooperativ-cuantice dintre atomi, biomolecule, cavități optice sub acțiunea radiației electromagnetice și aplicarea acestora în biofotonică pentru elaborarea echipamentelor moderne de decontaminare și diagnostica. Pe baza rezultatelor acestor studii, au fost propuse spre brevetare două dispozitive de decontaminare: unul se referă la dezinfecția lichidelor infectate, celălalt la sterilizarea instrumentarului chirurgical și de laborator. Ambele idei au obținut aviz pozitiv fiind introduse in registrul AGEPI cu numerele de depozit "s 2023 0031" respectiv "s 2024 0049".

SUMMARY

of the doctoral thesis "Cooperative quantum action of short radiation pulses with biomolecules during their propagation through metamaterials with its application in diagnostics, treatment and inactivation of pathogens", presented by Munteanu Ion for conferring the PhD degree in Physics at the specialty 131.01 "Mathematical Physics".

Structure of the thesis: The thesis was elaborated at the Institute of Applied Physics, State University of Moldova, Chisinau, 2025, is written in Romanian and consists of introduction, four chapters, general conclusions and recommendations, 135 bibliographic titles, 122 pages of basic text, 46 figures. The results presented in the thesis are published in 15 scientific papers. Based on the developed theories, two patents were obtained, and another is in the process of being obtained.

Key words: pulsed UV-C radiation, quantum effects, metamaterials, decontamination, DNA dimerization, pathogen inactivation.

Research area: biophysics, nonlinear optics and quantum optics.

The aim of the thesis: The purpose of the thesis is to present the results of research on the cooperative quantum action of short pulses of UV-C radiation during their propagation through metamaterials for the inactivation of pathogens.

Objectives of the thesis: analysis of the interaction between UV-C radiation and matter; inactivation of pathogens due to the applied pulsed coherent UV-C radiation; the nonlinear description of the dependence of the DNA/RNA dimerization rate on the applied ultraviolet C radiation in the form of short pulses is proposed; application of the Born-Oppenheimer model to DNA dimerization under the action of radiation; manipulation of biomolecules using rotation channels through metamaterials penetrated by UVC radiation; the possibility of applying these concepts is proposed; decontamination equipment with dispersion of radiation in volume through spherical fiber/metamaterial in the disinfection of fluids (air, water, blood serum, etc.); the possibilities of applying and optimizing the intensity of UVC radiation applied in the proposed decontamination equipment on the volume of metamaterial bases are studied.

Scientific novelty and originality: For the first time, it was proposed to channel UV-C radiation through various special optical systems (metamaterials) using different types of fibres/balls quartz combinations. In the experimental investigations, the penetration depth of UV-C radiation through such metamaterial packagings at different intensities was determined, as well as the dependence of the radiation dose on the inactivation rate of the yeast solution. Two patent applications were proposed for patenting: a liquid decontamination device and a UV-C sterilizer.

The solved scientific problem: consists in highlighting an efficient inactivation mechanism based on theoretical and experimental research, taking into account their correlation.

Theoretical Significance: of the thesis consists in the development of the theory in the Born-Opingheimer model (approximation) and its application to DNA dimerization under the action of ultraviolet C radiation, including the development of technologies for the decontamination of pathogens using short radiation pulses propagated through metamaterials to increase the decontamination rate of infected solutions. Since the electronic subsystem is faster compared to the nuclear subsystem of biomolecules, the solution of the quantum excitation problem of the electronic subsystem is investigated, considering that the atomic subsystem of nuclei is slow and can be considered fixed.

Application value: This implies the possibility of applying the research results described in the thesis for the development and elaboration of decontamination devices with a high rate of inactivation of pathogens, present in different environments such as: water, air and surfaces.

Implementation of scientific results: The results obtained were used within the institutional project within the State Program (2020-2023) ANCD Project 20.80009.5007.01: Quantum cooperativity between emitters (nuclei, atoms, quantum dots, molecules, biomolecules, metamaterials) and its application in informatics, advanced biophotonics optogenetics, as well as within the subprogram 011206: Cooperative-quantum phenomena between atoms, biomolecules, optical cavities under the action of electromagnetic radiation and their application in biophotonics for the development of modern decontamination and diagnostic equipment. Based on the results of these studies, two decontamination devices were proposed for patenting: one refers to the disinfection of infected liquids, the other to the sterilization of surgical and laboratory instruments. Both ideas obtained a positive opinion and were entered in the AGEPI register with the deposit numbers "s 2023 0031" and "s 2024 0049" respectively.

АННОТАЦИЯ

К докторской диссертации **«Кооперативное квантовое взаимодействие коротких импульсов излучения с биомолекулами при их распространении через метаматериалы с применением его в диагностике, лечении и инактивации патогенов»**, представленной Munteanu Ion, для получения ученой степени доктора физических наук по специальности 131.01 «Математическая физика», Кишинев 2025.

Структура диссертации: Диссертация была выполнена в Институте Прикладной Физики, Кишинёв,2025, написана на румынском языке и состоит из введения, 4 глав, общих выводов и рекомендаций, 135 библиографических названий, 122 страниц основного текста, 46 рисунков. Результаты, представленные в диссертации, опубликованы в 15 научных статьях.

Ключевые слова: импульсное УФ-С-излучение, метаматериалы, квантовые эффекты, димеризация ДНК, инактивация патогенов.

Сфера научных интересов: биофизика, нелинейная оптика и квантовая оптика.

Основная цель диссертации: Целью диссертации является представление результатов исследований кооперативного квантового действия коротких импульсов УФ-С-излучения при их распространении через метаматериалы для инактивации патогенов.

Цели диссертации: анализ взаимодействия УФ-С-излучения с веществом; инактивация патогенов за счет применяемого когерентного импульсного УФ-С-излучения; предложено нелинейное описание зависимости скорости димеризации ДНК/РНК от приложенного короткоимпульсного ультрафиолетового излучения С; применение модели Борна-Оппенгеймера к димеризации ДНК под действием радиации; манипулирование биомолекулами с использованием вращательных каналов через метаматериалы, проницаемые для УФ-С-излучения; предложена возможность применения данных концепций для оборудования дезактивации с рассеиванием излучения в объеме через сферическое волокно/метаматериал при дезинфекции жидкостей (воздуха, воды, сыворотки крови и т.п.); Изучены возможности применения и оптимизации интенсивности УФС-излучения, применяемого в предлагаемом дезактивационном оборудовании на основе объемных метаматериалов.

Научная новизна и оригинальность: Впервые было предложено направлять УФ-С-излучение через различные специальные оптические системы (метаматериалы) с использованием различных типов комбинаций волокон и кварцевых шариков. В ходе экспериментальных исследований была определена глубина проникновения УФ-С-излучения через такую метаматериальную упаковку при различной интенсивности, а также зависимость дозы облучения от скорости инактивации дрожжевого раствора. Разработаны и запатентованы устройство для обеззараживания жидкости и стерилизатор УФ-С.

Решенная научная проблема: заключается в выделении эффективного механизма инактивации на основе теоретических и экспериментальных исследований с учетом их взаимосвязи.

Теоретическое значение диссертации: заключается в развитии теории в модели Борна-Опинггеймера (приближение) и ее применении к димеризации ДНК под действием ультрафиолетового излучения С, в том числе при разработке технологий дезактивации патогенов с использованием коротких импульсов излучения, распространяемых через метаматериалы, для повышения скорости дезактивации инфицированных растворов. Поскольку электронная подсистема является более быстрой по сравнению с ядерной подсистемой биомолекул, исследуется решение задачи квантового возбуждения электронной подсистемы, учитывая, что атомная ядерная подсистема является медленной и ее можно считать неподвижной.

Прикладное значение: Это предполагает возможность применения результатов исследований, описанных в диссертации, для разработки и создания дезактивационных устройств с высокой степенью инактивации патогенов, присутствующих в различных средах, таких как: вода, воздух и поверхности.

Внедрение научных результатов: Полученные результаты использованы в институциональном проекте в рамках Государственной программы (2020-2023) АНКО Проект 20.80009.5007.01: Квантовая кооперативность между излучателями (ядрами, атомами, квантовыми точками, молекулами, биомолекулами, метаматериалами) и ее применение в информатике, перспективной биофотонике, оптогенетике, а также в рамках подпрограммы 011206: Кооперативно-квантовые явления между атомами, биомолекулами, оптическими резонаторами под действием электромагнитного излучения и их применение в биофотонике для разработки современного дезактивационного и диагностического оборудования. По результатам этих исследований предложено к патентованию два дезактивационных устройства: одно относится к дезинфекции инфицированных жидкостей, другое - к стерилизации хирургических и лабораторных инструментов. Обе идеи получили положительное заключение и были внесены в реестр AGEPI с номерами депозитов «s 2023 0031» и «s 2024 0049» соответственно.

MUNTEANU ION

QUANTUM COOPERATIVE ACTION OF SHORT RADIATION PULSES WITH BIOMOLECULES DURING THEIR PROPAGATION THROUGH METAMATERIALS WITH ITS APPLICATION IN DIAGNOSTICS, TREATMENT AND INACTIVATION OF PATHOGENS

131.01. MATHEMATICAL PHYSICS

Summary of the PhD thesis in physical sciences

Approved for printing: September 04, 2025 | Paper format: 60×84 1/16
Offset paper. Offset printing. | Edition: 50 copies
Printing sheets: 2.0 | Order No. 00016

ProEdit SRL
1/1 Sprâncenoaia Street, MD-2028
Chișinău, Republic of Moldova