МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "MATHEMATICAL AND PHYSICAL MODELS OF QUANTUM AND NEURAL NETWORKS", Part 4. (Training of PhD students of the specialty: 113 – "Applied mathematics" and others)

«Затверджено» на засіданні групи забезпечення спеціальності Дородова групи Кецеліус О.Ю. «Затверджено» на засіданні кафедри вищої та прикладної математики Протокол №1 від 28/08/2021 Зав. кафедри Кафедри Вищої та прикладної математики

Одеса 2021

THE MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE ODESSA STATE ENVIRONMENTAL UNIVERSITY

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "MATHEMATICAL AND PHYSICAL MODELS OF QUANTUM AND NEURAL NETWORKS", Part 4. УДК 584.2 G31 ББК 23.131

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "MATHEMATICAL AND PHYSICAL MODELS OF QUANTUM AND NEURAL NETWORKS, Part 4. (Training specialty: 113 - "Applied mathematics" and others)

Compiler:

Glushkov O.V., D.f.-m.s.(Hab.Dr.), prof., Head of the department of higher and applied mathematics (OSENU)

Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Svinarenko A.A., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Ignatenko a.V., C.f.-m.s.(PhD), assoc.-prof. of the department of higher and applied mathematics (OSENU)

Editor:

Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Reviewer:

P'yanova I.Yu., c.phil.s. (PhD), assoc.-prof., Head of the department of Foreign Languages (OSENU)

PREFACE

Discipline "MATHEMATICAL AND PHYSICAL MODELS OF QUANTUM AND NEURAL NETWORKS " is an elective discipline in the cycle of professional training of graduate students (third level of education) in the specialty 113- Applied Mathematics.

It is aimed at mastering (providing) a number of planned competencies, including the study of the modern apparatus of quantum and neural networks and on their basis to build new computational algorithms and software systems for mathematical modeling of linear and nonlinear processes in complex systems with regular and chaotic dynamics

The place of the discipline in the structural and logical scheme of its teaching: the knowledge gained in the study of this discipline is used in writing dissertations, the subject of which is related to the study of properties and regular and chaotic dynamics of various [classes of mathematical, physical chemical, cybernetic, socio-economic and environmental systems. The basic concepts of the discipline are the desired toolkit of an experienced specialist in the field of applied mathematics.

The purpose of studying the discipline is to master (provide) a number of competencies, in particular, the ability to develop new and improve existing mathematical and physical models of quantum and neural networks and build new computational algorithms and software for mathematical modeling of linear and nonlinear processes in complex systems. regular and chaotic dynamics.

After mastering this discipline, the graduate student must be able to improve existing modern mathematical and physical models of quantum and neural networks, as well as build new efficient models, and on their basis to develop new computational algorithms and software for analysis, mathematical modeling and prediction of linear and nonlinear processes in complex systems with regular and chaotic dynamics.

The study of the discipline "Mathematical and Physical Models of Quantum and Neural Networks" is conducted in the second year of study (4th semester; full-time and part-time forms of study) and includes lectures and practical classes. Types of control of current knowledge - tests and term papers, surveys, tests.

Topics of these issue: Quantum neural network and finding the minimum of some objective function by nonstationary evolution of the quantum system.

Mathematical and physical models of quantum neural networks. Paradigm of quantum chaotic computations. Modeling of systems described by the Schrödinger equation.

Topic: Quantum neural network and finding the minimum of some objective function by nonstationary evolution of the quantum system. Mathematical and

physical models of quantum neural networks. Paradigm of quantum chaotic computations. Modeling of systems described by the Schrödinger equation. **Торіс 3Б- Л4 :** Квантова нейронна мережа і пошук мінімуму деякої

цільової функції шляхом нестаціонарної еволюції квантової системи. Математичні та фізичні моделі квантових нейромереж. Парадігма квантових хаотичних обчислень. Моделювання систем, що описуються рівнянням Шредінгеру.

Introduction

In the last decade, the theory of dynamical systems and the theory of chaos are characterized by significant progress both in the development of new concepts, as well as new methods and new applications. Modern theory of nonlinear dynamical systems has established the main mechanisms of instability and scenarios of transition to chaos in many nonlinear classical systems and devices with many applications in various sciences, including mechanics, chemistry, biology, physics and others.

In real, especially quantum systems, chaotic dynamics take much more complex, partially or not completely understood forms. According to modern concepts, the theory of quantum chaos actually studies quantum-mechanical systems that are chaotic in the classical limit.

Traditionally, quantum chaos refers to the set of effects observed in quantumphysical systems relating to purely nonlinear effects, which are manifested in quantum systems described by equations of the Schrödinger type or density matrix. It is well known that quantum mechanics, which has existed for over 60 years, allows us to describe both systems that integrate in the classical limit (such as a hydrogen atom) and classically unintegrated systems (such as a helium atom).

The well-known principle of correspondence indicates that quantum mechanics in the quasiclassical domain at scales of the system comparable to the de Broglie wavelength continuously goes to the classical one. On the other hand, in quantum mechanics, the concept of trajectory, at least in pragmatic or Copenhagen interpretation, loses its usual meaning (it reappears only in the quasiclassical domain).

There is an opinion that in the interpretation of the phenomenon of quantum

chaos it is more correct to speak about such characteristic manifestations as the intersection of energy levels in multivariable space, elements of stochasticity in the spectra of particularly highly excited states of atomic and molecular systems, phenomena of clustering states, interference, fluctuations, and merging of resonances etc. From the other side, it was considered the most natural study of the phenomenon of chaos on the basis of methods of classical mechanics and qualitative theory of differential equations, within which it is natural to operate concepts such as bifurcation, instability, boundary cycle, strange attractor, etc. [1-18].

Their application to quantum systems is also quite acceptable, moreover, often the scenario of emergence of a chaotic dynamics in quantum models is (not always) similar to the classical one. r example, the stochastic motion of an electron in an atom in the external fields is naturally interpreted in the language of consideration of a certain type of resonance interactions of modes corresponding to the motion in these fields, and its manifestation area narrows as an interaction increases.

The qualitative picture of the process of emerging chaotic dynamics in quantum systems in general is reduced to the following scenario: an external, for example, a magnetic field leads to the appearance of primary nonlinear resonances, a strong interaction between which leads to the appearance of secondary resonances and the emergence of stochastic oscillations, right down to the formation of the Arnold's web. When the external field strength is above a certain critical value, the various stochastic layers merge, resulting in global stochasticity in the system.

An analysis of the chaotic phenomena in quantum systems was carried out not only based on the methods of classical mechanics (in fact, within the framework of the Newtonian dynamics), but also on the basis of semiclassical or semiquantum methods, in particular, the method of quantum trajectories (quantization of classical mechanics), and path integrals by Feynman-Higgs, the Gutswiller's theory of "periodic orbits", the Delos closed orbit method, complex coordinate method, a random matrix theory, diagonalization methods and some others (c.g. [1-8]). New field of investigations of chaotic effects in theory of quantum systems has been provided by a great progress in a development of a chaos and dynamical systems theory methods [6-22].

In previous our papers [7,8,17-19] we have presented a few new computational quantum algorithms to study stochastic futures and chaotic elements in dynamics of atomic and molecular systems in an external electromagnetic fields. The known mathematical tools such as power spectrum analysis, correlation integral and fractal algorithms, the Lyapunov's exponents analysis and others have been applied to numerical analysis of chaotic features in dynamics of the quantum systems.

Here it is presented an effective mathematical approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic and molecular systems in an electromagnetic field as mathematical and physical principal basis for quantum models of quantum neural networks. Paradigm of quantum chaotic computations is outlines. Modeling of systems described by the Schrödinger equation is used to treat a chaotic dynamics of systems.

It is proposed the theoretical scheme that includes new quantum-dynamic models (based on the finite-difference solution of the Schrödinger equation, optimized operator perturbation theory and realistic model potential method) and advanced nonlinear analysis and a chaos theory methods such as power spectrum analysis, the correlation integral algorithm, the Lyapunov's exponents and Kolmogorov entropy analysis etc. The approach is applied to study of chaotic phenomena in some atomic and diatomic systems in an external electromagnetic (magnetic) field.

Mathematical and physical principal basis for quantum models of quantum neural networks. A quantum-geometric approach to quantum systems in electromagnetic field

In the Refs. [7,8,17-19] we have given a review of new methods and algorithms of the chaos-geometric approach to analysis, processing, modeling and forecasting a chaotic dynamics for different classical and quantum systems.

So, here we pay attention only at main elements. The total scheme for studying chaos-dynamical phenomena in quantum systems (in particular, atomic systems in magnetic, crossed electric and magnetic fields, Rydberg atoms in a electromagnetic field, molecular systems in a infrared electromagnetic field etc) and computing the topological and dynamical invariants in application to quantum systems include the following:

A) Quantum-dynamical computing of quantum systems: Schrödinger (Dirac) equation for quantum system in an external field (numerical solving, the finite differences , model potential , operator perturbation theory etc methods); Preliminary analysis and processing dynamical variable series of physical system;

B) Preliminary study and assessment of the presence of chaos: the Gottwald-Melbourne test; Fourier decompositions, irregular nature of change – chaos; Spectral analysis, Energy spectra statistics, the Wigner distribution, the spectrum of power, "Spectral rigidity";

C) The multi-fractal geometry: computation time delay τ using autocorrelation function or mutual information; Determining embedding dimension by the method of correlation dimension or algorithm of false nearest neighbouring points; Calculation of multi-fractal spectra; wavelet analysis;

D) Computing global Lyapynov's exponents, Kaplan-York dimension, Kolmogorov entropy, average predictability measure; Methods of nonlinear prediction (classical and quantum neural network algorithms, the algorithm optimized trajectories, stochastic propagators, memory functions etc...;

The key idea in the study of the spectra of chaotic systems and, in particular, quantum systems, is provided by the fact that a definition of quantum chaos is interpreted primarily as a property of a group of states of the spectra of the system. It is the interpretation of one of the mechanisms of quantum chaos through the induction of resonances in the spectrum of the system, their strong interaction with subsequent overlapping, the emergence of stochastic layers and further transition to a global stochasticity in the system.

It has led to the most common criterion for chaos in spectral research (especially from the point of view of the mechanism of overlapping and merging of resonances), i.e. the criterion of a chaos by Chirikov.

In this scheme, the overlap of nonlinear resonances is defined as the ratio of the sum of the half-widths of the resonances to the distances between them

$$K = \left[(\Gamma_1/2) + (\Gamma_1/2) \right] / |E_2 - E_1|, \tag{1}$$

where $\Gamma_i \operatorname{Ta} E_i$ are, respectively, the width and energy of the "i" -th resonance. It is usually assumed that at sufficiently large values ($K \ge 4$) the phenomenon of chaos is realized in the system.

Among the spectral characteristics, which are usually calculated when studying the elements of chaos in the spectra of systems, one should include: 1) The relative value of the interlevel distances s_n , which is standardly defined as:

$$S_n = (E_n - E_{n-1})\rho(E_n),$$
 (2)

where $\rho(E)$ is a density of levels.

2) Function P (S) of the distribution of the relative value of the interlevel distances s_n ;

if the position of the levels in the spectrum is not chaotic, then P(S), as a rule, has the form of a Poisson distribution $P_p(S) = \exp(-S)$; if there is chaos in the system, then the Wigner-Dyson distribution is realized (in general, the Brody distribution).

3) Characteristics of the degree of ordering of levels in the spectrum at large (in comparison with the interlevel distance) ε the spectral stiffness $\Delta_{a}(L)$, which is defined as follows:

$$\Delta_{3}(x,L) = \frac{1}{L} \min_{A,B} \int_{x}^{x+L} (n(\varepsilon) - A\varepsilon - B)^{2} d\varepsilon$$
(3)

It should be borne in mind that for a sequence of levels ε_n , normalized to a unit density ($\varepsilon_n = \varepsilon_{n-1} + S_n$), a step function $n(\varepsilon)$, equal to the number of levels with $\varepsilon_n \le \varepsilon$ is used.

By construction, $n(\varepsilon)$, has the form of a ladder with a single average slope. The value of $(\Delta_3(x, L))$, averaged over the values of x from the region in which the nature of the fluctuations of the spectrum can be considered constant, depends only on L and is denoted by $\Delta_3(L)$. The function $\Delta_3(L)$ describes the ordering of the spectrum over large areas: the slower the growth of $\Delta_3(L)$ with increasing L, the less probable in the spectrum are close clusters of levels and gaps with reduced level density.

4) Correlation coefficients C (n) values of energy intervals, divided by a fixed number of levels, determined in the usual way:

$$C(n) = \frac{\sum_{i} (S_{i-n}-1)(S_{i}-1)}{\left[\sum_{i} (S_{i+n}-1)^{2} \sum_{i} (S_{i}-1)^{2}\right]_{2}^{1}}.$$
 (4)

Finally, another of the most common characteristics of nonlinear (chaotic) dynamics is the so-called power spectrum, which is determined in a standard way.

More detailed characteristics of spectral methods are given, for example, in [7-19].

In Table 1 we present the main blocks of the combined quantum-dynamical and chaos-geometric approach to nonlinear analysis, modelling and prediction of chaotic dynamics of quantum system in an electromagnetic field.

Table 1. Combined quantum-dynamical and quantum-geometric approach to nonlinear analysis, modelling and prediction of chaotic dynamics of quantum (atomic, molecular and nuclear) system in an electromagnetic field.

I. Quantum-dynamical computing of quantum systems:

- Schrödinger (Dirac) equation for quantum system in an external field (numerical solving, the finite differences, model potential, operator perturbation theory etc methods)
- 2. Preliminary analysis and processing dynamical variable series of
 - physical system

∜

II. Study and assessment of the presence of chaos:

3. Fourier decompositions, irregular nature of change – chaos;

4. Spectral analysis, Energy spectra statistics, the Wigner distribution, the spectrum of power, "Spectral rigidity";

∜

III. The multi-fractal geometry of the phase space. :

- 5. Autocorrelation function and mutual information;
- 5. Method of correlation dimension
- 6. Wavelet analysis;

₩

- IV. Prediction model:
 - 6. Computing global Lyapynov indicators; Kaplan-York dimension,
- 7. Methods of nonlinear prediction.

In Refs. [7,8] the total approach has been used for studying the chaotic features in spectrum of the hydrogen atom in a magnetic field, diatomic molecules interacting with a linearly polarized electromagnetic field. It is shown that the chaotic features are realized in the nonlinear dynamics of diatomic molecules in a linearly polarized electromagnetic field that is in a reasonable agreement with the classical modelling data by Berman, Kolovskii, Zaslavsky, Zganh et al [1-5]. The detailed description of the every stage in the scheme (Table 1) is earlier presented in the Refs. [7,8,17-30]. All calculations are performed with using "Geomath", "Superatom", "Quantum Chaos", "ScanPoints" computational codes [7,9,17-19,31-44].

Chaotic dynamics of atoms and molecules in electromagnetic field: Numerical solution of the Schrödinger equation and power spectrum analysis

In this subsection we present the results of modeling the hydrogen and rubidium spectra in an external magnetic (crossed electric and magnetic) filed. In Ref. [7,8,18,44] it has been developed an effective nonperturbative quantum and chaos-dynamic approach to modeling the chaotic dynamics of atomic systems in homogeneous magnetic field, which is based on the operator optimized

perturbation theory and finite-difference solution of the Schrödinger equation for an atom in the field (in a cylindrical coordinate system $z||B; \Psi \sim e^{iM\varphi}$). The cited equation can be written as follows:

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2} - \frac{M^2}{\rho^2} - 4\gamma^2\rho^2 + \frac{4}{r} + V_c(r) + \left(\frac{E}{R_y} - \gamma M\right)\right]\Psi(\rho, z) = 0$$
(5)

where $\gamma = B/B_o$, $B_o = 2.3505 \cdot 105$ T, $V_c(r)$ – potential electron self-consistent field, including the Hartree potential plus the Kohn-Sham exchange-correlation potential (other notations are standard).

The quantitative modeling of regular and chaotic dynamics, computation power and spectral parameters for the atoms of hydrogen, neon in a uniform magnetic field ($\gamma = 0.01$ -10000) showed that the system generated quantum chaos, which is manifested in a very complex and irregular dependences of state energies upon the magnetic field amplitude, the presence of the level intersections (as example, for the Ne quasi-intersections in dependence of the energy states $|0_N\rangle$ and $|2p_0\rangle$ upon the magnetic field amplitude at $\gamma = 158.7$, $|2p_0\rangle$ and $|1s^2\rangle$ states- at γ =40.2), in a photoionization cross sections, power spectra etc.

We have calculated and carried our analysis of the photoionization spectrum, power spectrum, the energies and widths of resonances, the distribution of resonances in the hydrogen atom in the special magnetic field with the strength 5.96 T (the energy interval 20-80 cm⁻¹).

According to our data, the density of states in the middle of each channel (Landau resonances) is 33 cm⁻¹ for the average resonance width - 0.004 cm⁻¹, which is consistent with experimental data Kleppner et al: 0.004-0.006cm⁻¹ (c.g. [7,8,18,44]).

Further we present the results of modelling the chaotic dynamics of atomic systems in the crossed electric F_1 and magnetic γ fields, based on the numerical solution of the Schrödinger equation:

$$H = \frac{1}{2}(p_{\rho}^{2} + l_{z}^{2} / \rho^{2}) + \frac{1}{2}(2 + \frac{1}{8})\gamma^{2}\rho^{2} + \frac{1}{2}p_{z}^{2} + F_{1}z \cdot \sin(\omega t) + V(r)$$
(6)

the operator perturbation theory and density functional method [18,44].

Here we use the following denotations:

$$\widetilde{f} = F_1 \gamma^{-4/3}, \ \mathcal{E} = E^{ion} \gamma^{-2/3},$$

where E^{ion} is an ionization energy of a free atom. We have carried out modelling a chaotic dynamics for the Rydberg Li, Rb (n ~ 100, m = 0) atoms in a static magnetic (B = 4.5T) and oscillating electric field with frequency $\omega = 102$ Mru ($\varepsilon = -0.03, \varpi = 0.32, \gamma - 1/3$ in the range 35-50; f = 0.000 - 0.070).

Figure 1 shows the power spectrum of Rb: a- in a magnetic field (f = 0, the electric field is absent); (b) in a static magnetic field and oscillating electric field f = 0.0035 (our data).



Fig. 1. The power spectrum of Rb: (a)- in a magnetic field (f = 0, the electric field is absent); (b) in static magnetic field and oscillating electric field f = 0.0035 (our data).

The scenario of transition to chaos in the system includes the induction of nonlinear resonances by a magnetic field, their strong interaction and further merging with the appearance of global chaos when critical field strength is exceeded.

Further we shortly present the advanced data for the modeling the temporal dynamics (polarization parameter) of the diatomic molecule PbO in the resonant electromagnetic field. This molecule in the linearly polarized field has been studied, for example, in ref. [7,8]. All information about the key characteristics of electromagnetic field as well as spectral molecule parameters is listed in the cited Refs. The new element here is using more efficient approach to solving the Schrödinger equation with the realistic density functional theory potential curve of diatomic molecule U(x) [7,8]. We numerically studied the corresponding temporal dependence of a polarization (which is normalized to the intensity of the field interaction with the molecule) on the basis of the quantum-geometric approach to analysis of a chaotic dynamics of the molecule interacting with a resonant linearly polarized field.

The concrete step is an analysis of the corresponding time series with the $n=7.6\cdot10^3$ and $\Delta t=5\cdot10^{-14}$ s.

In Table 2 we list the computed values of the correlation dimension D_c , the Kaplan-York attractor dimension (D_L) , the Lyapunov's exponents $(L_i, i=1-3)$, the Kolmogorov entropy (KE). In conclusion of this subsection let us underline, that difference between the presented data and data of the Ref. [8] on the

Table 2. The correlation dimension D_c , Lyapunov's exponents (L_i , *i*=1,2), Kaplan-York attractor dimension (D_L), Kolmogorov entropy (KE)

D _c	L_1	L_2	D_L	KE
2.83	0.153	0.0185	2.58	0.172

topological and dynamical invariants can be explained by processing different polarization time series.

Concluding remarks

Here it is presented an effective mathematical approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic systems in an electromagnetic field as mathematical and physical principal basis for quantum models of quantum neural networks. Paradigm of quantum chaotic computations is outlined.

Modeling of systems described by the Schrödinger equation is used to treat a chaotic dynamics of systems. We presented the fundamentals of a computational approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic systems in an electromagnetic field. To treat chaotic dynamics of systems it is constructed effective scheme that includes new quantum-dynamic models (based on the finite-difference solution of the Schrödinger equation, optimized operator perturbation theory and realistic model potential for quantum systems) and advanced analysis methods of dynamical systems and chaos theory. As illustration we presented some numerical results for atoms of hydrogen and rubidium in a magnetic and crossed magnetic and oscillating electric field. The numerical values for a set of dynamical and topological invariants are listed.

2. Task options for self-sufficient work

Task Option 1.

1). Give the key definitions: Quantum neural network and finding the minimum of some objective function by nonstationary evolution of the quantum system. Mathematical and physical models of quantum neural networks. Paradigm of quantum chaotic computations. Modeling of systems described by the Schrödinger equation.

2). Propose the key elements of mathematical approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic systems in an electromagnetic field as mathematical and physical principal basis for quantum models of quantum neural networks. Propose your paradigm of quantum neural networks chaotic computations.

3). Construct quantum-dynamic models (based on the finite-difference solution of the Schrödinger equation, optimized operator perturbation theory and realistic model potential for quantum systems) and advanced analysis methods of dynamical systems and chaos theory.

4). Perform numerical modelling for atoms of **hydrogen and sodium** in a magnetic and crossed magnetic and oscillating electric field (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark"; necessary numerical parameters should be self-taken).

Task Option 2.

1). Give the key definitions: Quantum neural network and finding the minimum of some objective function by nonstationary evolution of the quantum system. Mathematical and physical models of quantum neural networks. Paradigm of quantum chaotic computations. Modeling of systems described by the Schrödinger equation.

2). Propose the key elements of mathematical approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic systems in an electromagnetic field as mathematical and physical principal basis for quantum models of quantum neural networks. Propose your paradigm of quantum neural networks chaotic computations.

3). Construct quantum-dynamic models (based on the finite-difference solution of the Schrödinger equation, optimized operator perturbation theory and realistic model potential for quantum systems) and advanced analysis methods of dynamical systems and chaos theory.

4). Perform numerical modelling for atoms of **hydrogen and rubidium** in a magnetic and crossed magnetic and oscillating electric field (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark"; necessary numerical parameters should be self-taken).

Task Option 3.

1). Give the key definitions: Quantum neural network and finding the minimum of some objective function by nonstationary evolution of the quantum system. Mathematical and physical models of quantum neural networks. Paradigm of quantum chaotic computations. Modeling of systems described by the Schrödinger equation.

2). Propose the key elements of mathematical approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic systems in an electromagnetic field as mathematical and physical principal basis for quantum models of quantum neural networks. Propose your paradigm of quantum neural networks chaotic computations.

3). Construct quantum-dynamic models (based on the finite-difference solution of the Schrödinger equation, optimized operator perturbation theory and realistic model potential for quantum systems) and advanced analysis methods of dynamical systems and chaos theory.

4). Perform numerical modelling for atoms of **hydrogen and caesium** in a magnetic and crossed magnetic and oscillating electric field (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark"; necessary numerical parameters should be self-taken).

Task Option 4.

1). Give the key definitions: Quantum neural network and finding the minimum of some objective function by nonstationary evolution of the quantum system. Mathematical and physical models of quantum neural networks. Paradigm of quantum chaotic computations. Modeling of systems described by the Schrödinger equation.

2). Propose the key elements of mathematical approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic systems in an electromagnetic field as mathematical and physical principal basis for quantum models of quantum neural networks. Propose your paradigm of quantum neural networks chaotic computations.

3). Construct quantum-dynamic models (based on the finite-difference solution of the Schrödinger equation, optimized operator perturbation theory and realistic model potential for quantum systems) and advanced analysis methods of dynamical systems and chaos theory.

4). Perform numerical modelling for atoms of **hydrogen and francium** in a magnetic and crossed magnetic and oscillating electric field (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark"; necessary numerical parameters should be self-taken).

Task Option 5.

1). Give the key definitions: Quantum neural network and finding the minimum of some objective function by nonstationary evolution of the quantum system. Mathematical and physical models of quantum neural networks. Paradigm of quantum chaotic computations. Modeling of systems described by the Schrödinger equation.

2). Propose the key elements of mathematical approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic systems in an electromagnetic field as mathematical and physical principal basis for quantum models of quantum neural networks. Propose your paradigm of quantum neural networks chaotic computations.

3). Construct quantum-dynamic models (based on the finite-difference solution of the Schrödinger equation, optimized operator perturbation theory and realistic model potential for quantum systems) and advanced analysis methods of dynamical systems and chaos theory.

4). Perform numerical modelling for atoms of **hydrogen and magnesium** in a magnetic and crossed magnetic and oscillating electric field (using Fortran Power Station, Version 4.0; PC Code: "Superatom-Stark"; necessary numerical parameters should be self-taken).

Task Option 6.

1). Give the key definitions: Quantum neural network and finding the minimum of some objective function by nonstationary evolution of the quantum system. Mathematical and physical models of quantum neural networks. Paradigm of quantum chaotic computations. Modeling of systems described by the Schrödinger equation.

2). Propose the key elements of mathematical approach to studying deterministic chaos and strange attractors in dynamics of nonlinear processes in atomic systems in an electromagnetic field as mathematical and physical principal basis for quantum models of quantum neural networks. Propose your paradigm of quantum neural networks chaotic computations.

3). Construct quantum-dynamic models (based on the finite-difference solution of the Schrödinger equation, optimized operator perturbation theory and realistic model potential for quantum systems) and advanced analysis methods of dynamical systems and chaos theory.

4). Perform numerical modelling for atoms of **hydrogen and lithium** in a magnetic and crossed magnetic and oscillating electric field (using Fortran Power Station , Version 4.0; PC Code: "Superatom-Stark" ;necessary numerical parameters should be self-taken).

References

- 1. Berman, G.P., Bulgakov, E.N., Holm, D.D.: Nonlinear resonance and dynamical chaos in a diatomic molecule driven by a resonant IR field. Phys. Rev. A 52, 3074-3080 (1995)..
- 2. Zhang, C., Katsouleas, T., Joshi, C.: Harmonic frequency generation and chaos in laser driven molecular vibrations. In Proc. of Shortwavelength Physics with Intense Laser Pulses, San-Diego, CA, March 29-31, 1993;
- 3. Zhai, Liang-Jun, Zheng, Yu-Jun, Ding, Shi-Liang: Dynamics of vibrational chaos and entanglement in triatomic molecules: Lie algebraic model. Chin. Phys. B. 21(7), 070503 (2012).
- 4. Lombardi, M., Matzkin, A.: Dynamical entanglement and chaos: The case of Rydberg molecules. Phys. Rev. A. 73, 062335 (2006).
- 5. Arango, C.A., Kennerly, W.W., Ezra, G.S.: Classical and quantum mechanics of diatomic molecules in tilted fields. J. Chem. Phys. 122, 184303 (2015).
- Glushkov, A.V., Prepelitsa, G.P., Svinarenko, A.A., Zaichko, P.A.: Studying interaction dynamics of the non-linear vibrational systems within non-linear prediction method (application to quantum autogenerators). In: Awrejcewicz, J., Kazmierczak, M., Olejnik, P., Mrozowski J. (eds.) Dynamical Systems Theory, T1, pp. 467–477. Lodz Univ. Press., Lodz (Poland) (2013).
- 7. Glushkov, A.V., Buyadzhi, V.V., Kvasikova, A.S., Ignatenko, A.V., Kuznetsova, A.A., Prepelitsa, G.P., Ternovsky, V.B.: Nonlinear chaotic dynamics of Quantum systems: Molecules in an electromagnetic field and laser systems. In: Tadjer, A., Pavlov, R., Maruani, J., Brändas, E., Delgado-Barrio, G. (eds.) Quantum Systems in Physics, Chemistry, and Biology. Series: Progress in Theoretical Chemistry and Physics (Book 30), pp. 71-84. Springer (2016).
- Ignatenko A.V., Buyadzhi A.A., Buyadzhi V.V., Kuznetsova A.A., Mashkantsev A.A., Ternovsky E.V.: Nonlinear Chaotic Dynamics of Quantum Systems: Molecules in an Electromagnetic Field. In: Jenkins, S., Kirk, S. R., Maruani, J., Brändas E. (eds.) Advances in Quantum Chemistry, vol. 78, pp. 149–170. Elsevier (2019).
- 9. Gottwald, G., Melbourne, I.: Testing for chaos in deterministic systems with noise. Physica D. 212 ,100–110 (2005).
- 10. Packard, N.H., Crutchfield, J.P., Farmer, J.D., Shaw, R.S.: Geometry from a time series. Phys. Rev. Lett. 45, 712–716 (1980).
- Kennel, M.B., Brown, R., Abarbanel, H.: Determining embedding dimension for phase-space reconstruction using a geometrical construction. Phys. Rev. A 45, 3403–3411 (1992).
- 12. Abarbanel, H.D.I., Brown, R., Sidorowich, J.J., Tsimring, L.Sh.: The analysis of observed chaotic data in physical systems. Rev. Mod. Phys. 65, 1331–1392 (1993).

- 13. Schreiber, T.: Interdisciplinary application of nonlinear time series methods. Phys. Rep. 308, 1–64 (1999).
- 14. Fraser, A.M., Swinney, H.L.: Independent coordinates for strange attractors from mutual information. Phys. Rev. A. 33, 1134–1140 (1986).
- 15. Grassberger, P., Procaccia, I.: Measuring the strangeness of strange attractors. Physica D.9, 189–208 (1983).
- 16. Gallager, R.G.: Information theory and reliable communication. Wiley, N-Y. (1986).
- 17. Glushkov, A.V.: Methods of a chaos theory. Astroprint, Odessa (2012).
- 18. Glushkov, A.V.: Relativistic Quantum theory. Quantum Mechanics of Atomic Systems. Astroprint, Odessa (2008).
- 19. Glushkov, A.V., Svinarenko, A.A., Loboda, A.V.: Theory of neural networks on basis of photon echo and its program realization. TEC, Odessa (2003).
- Khetselius, O.Yu.: Forecasting evolutionary dynamics of chaotic systems using advanced non-linear prediction method. In: Awrejcewicz, J., Kazmierczak, M., Olejnik, P., Mrozowski J. (eds.) Dynamical Systems Applications, T2, pp. 145–152. Lodz Univ. Press., Lodz (Poland) (2013).
- Bunyakova, Yu.Ya., Ternovsky, V.B., Dubrovskaya, Yu.V., Ignatenko, A.V., Svinarenko, A.A., Vitavetskaya, L.A.: Analysis of the beryllium-7 activity concentration dynamics in the atmospheric environment time series after the Fukushima Daiichi nuclear power plants emergency. Sensor Electr. and Microsyst. Techn. 14(4), 73–82 (2017).
- Khetselius, O.Yu., Brusentseva, S.V., Tkach, T.B.: Studying interaction dynamics of chaotic systems within non-linear prediction method: In: Awrejcewicz, J., Kazmierczak, M., Olejnik, P., Mrozowski J. (eds.) Application to neurophysiology. Dynamical Systems Applications, T2, pp. 251–259. Lodz Univ. Press., Lodz (Poland) (2013).
- Svinarenko, A.A., Ignatenko, A.V., Ternovsky, V., Nikola, L., Seredenko, S.S., Tkach, T.B.: Advanced relativistic model potential approach to calculation of radiation transition parameters in spectra of multicharged ions. J. Phys.: Conf. Ser. 548, 012047 (2014).
- 24. Florko, T.A., Ambrosov, S.V., Svinarenko, A.A., Tkach, T.B.: Collisional shift of the heavy atoms hyperfine lines in an atmosphere of the inert gas. J. Phys.: Conf. Ser. 397, 012037 (2012).
- 25. Buyadzhi, V.V., Zaichko, P.A., Gurskaya, M.Y., Kuznetsova, A.A., Ponomarenko, E.L., Ternovsky, V.B.: Relativistic theory of excitation and ionization of Rydberg atomic systems in a Black-body radiation field. J. Phys.: Conf. Ser. 810, 012047 (2017).
- 26. Svinarenko A.A., Khetselius O.Yu., Buyadzhi V.V., Florko T.A., Zaichko P.A., Ponomarenko E.L.: Spectroscopy of Rydberg atoms in a Black-body radiation field: Relativistic theory of excitation and ionization. Journal of Physics: C Series 548, P. 012048 (2014).

- 27. Khetselius, O.Yu.: <u>Hyperfine structure of atomic spectra.</u> Astroprint, Odessa (2008).
- 28. Khetselius, O.Yu.: <u>Quantum structure of electroweak interaction in heavy</u> <u>finite Fermi-systems</u>. Astroprint: Odessa (2011).
- 29. Khetselius, O.Yu.: Spectroscopy of cooperative electron-gamma-nuclear processes in heavy atoms: NEET effect. J. Phys.: Conf. Ser. 397, 012012 (2012).
- 30. Khetselius, O.Yu.: Atomic parity non-conservation effect in heavy atoms and observing P and PT violation using NMR shift in a laser beam: To precise theory. *J. Phys.: Conf. Ser.* 194, 022009 (2009).
- 31. Khetselius, O.Yu.: Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes. Int. J. Quant. Chem. 109, 3330–3335 (2009).
- 32. Khetselius, O.Yu.: Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes. Phys. Scripta. 135, 014023 (2009).
- 33. Khetselius, O.Yu.: <u>Relativistic Calculating the Spectral Lines Hyperfine</u> <u>Structure Parameters for Heavy Ions</u>. AIP Conf. Proc. 1058, 363–365 (2008).
- 34. Khetselius, O.Yu.: Relativistic Hyperfine Structure Spectral Lines and Atomic Parity Non-conservation Effect in Heavy Atomic Systems within QED Theory. AIP Conf. Proceedings 1290(1), 29-33 (2010).
- 35. Svinarenko, A.A.: Study of spectra for lanthanides atoms with relativistic many-body perturbation theory: Rydberg resonances. J. Phys.: Conf. Ser. 548, 012039 (2014).
- 36. Florko, T., Ambrosov, S., Svinarenko, A., Tkach, T.: Collisional shift of the heavy atoms hyperfine lines in an atmosphere of the inert gas. J. Phys.: Conf. Ser. 397, 012037 (2012).
- 37. Buyadzhi V.V., Kuznetsova A.A., Buyadzhi A.A., Ternovsky E.V., Tkach T.B.: Advanced Quantum Approach in Radiative and Collisional Spectroscopy of Multicharged Ions in Plasmas. In: Jenkins, S., Kirk, S. R., Maruani, J., Brändas E. (eds.) Advances in Quantum Chemistry, vol. 78, pp. 171–191. Elsevier (2019).
- 38. Dubrovskaya Yu.V., Khetselius O.Yu., Vitavetskaya L.A., Ternovsky V.B., Serga I.N.: Quantum Chemistry and Spectroscopy of Pionic Atomic Systems With Accounting for Relativistic, Radiative, and Strong Interaction Effects. In: Jenkins, S., Kirk, S. R., Maruani, J., Brändas E. (eds.) Adv. in Quantum Chemistry, vol. 78, pp. 193-222. Elsevier (2019).
- 39. Khetselius O.Yu.: Optimized Relativistic Many-Body Perturbation Theory Calculation of Wavelengths and Oscillator Strengths for Li-like Multicharged Ions. In: Jenkins, S., Kirk, S. R., Maruani, J., Brändas E. (eds.) Advances in Quantum Chemistry, vol. 78, pp. 223–251. Elsevier (2019).
- 40. Glushkov, A.V., Efimov, V.A., Gopchenko, E.D., Dan'kov, S.V., Polishchyuk, V.N., Goloshchak, O.P.: <u>Calculation of spectroscopic</u>

characteristics 4 of alkali-metal dimers on the basis of a model perturbation theory. Optics and Spectr. 84(5), 670–678 (1998).

- 41. Glushkov, A.V., Malinovskaya, S.V., Loboda, A.V., Shpinareva, I.M., Prepelitsa, G.P.: Consistent quantum approach to new laser-electron-nuclear effects in diatomic molecules. J. Phys.: Conf. Ser. 35, 420-424 (2006).
- 42. Glushkov, A.V.: Relativistic multiconfiguration time-dependent selfconsistent-field theory for molecules. Sov. Phys. Journal. 34(10), 871–876 (1991).
- 43. Glushkov A.V. Atom in an electromagnetic field; KNT: Kiev, 2005.
- 44. Huber, K.P.; Herzberg, G. Molecular spectra and molecular structure. IV. Constants of Diatomic Molecules; Van Nostrand Reinhold Co.: New York, **1979**.

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "MATHEMATICAL AND PHYSICAL MODELS OF QUANTUM AND NEURAL NETWORKS", Part 4. (Training specialty: 113 - "Applied mathematics" and others)

Compiler:

Glushkov O.V., D.f.-m.s.(Hab.Dr.), prof., Head of the department of higher and applied mathematics (OSENU)

Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Svinarenko A.A., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Ignatenko a.V., C.f.-m.s.(PhD), assoc.-prof. of the department of higher and applied mathematics (OSENU)

Editor:

Khetselius O.Yu., D.f.-m.s.(Hab.Dr.), prof., prof. of the department of higher and applied mathematics (OSENU)

Reviewer:

P'yanova I.Yu., c.phil.s. (PhD), assoc.-prof., Head of the department of Foreign Languages (OSENU)

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