THE MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE

ODESSA STATE ENVIRONMENTAL UNIVERSITY

Methodical instructions for practical work of PhD students, tests performance and distance learning in the discipline «Fractal geometry and a chaos theory», Part 5

«Затверджено»
на засіданні групи забезпечення спеціальності
Протокол №1 від 28/08/2021 Голова групи Хецеліус О.Ю.

«Затверджено»
на засіданні кафедри вищої та прикладної математики
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Methodical instructions for practical work of PhD students, tests performance and distance learning in the discipline «Fractal geometry and a chaos theory», Part 5

Odessa 2021

Methodical instructions for practical work of the second-year PhD students and tests performance in the discipline «Fractal Geometry and Theory of a Chaos», Part 5
(Training specialty – 113 “Applied Mathematics” and others)

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PREFACE

The discipline "Fractal geometry and the theory of chaos" is a selective discipline in the cycle of professional training for postgraduate (PhD) students (third level of education) in specialty 113- Applied Mathematics.

It is aimed at assimilating (assuring) a number of planned competencies, including the study of the modern apparatus of fractal geometry and chaos theory, as well as new methods and algorithms of mathematical physics of complex chaotic systems with possible generalizations on various classes of mathematical, physical-chemical, cybernetic, socio-economic and ecological systems, the use of modern scientific methods and the achievement of scientific results that create potentially new knowledge in the theory and practice of chaotic phenomena.

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

The purpose of studying the discipline is the assimilation (assurance) of a number of competencies, in particular, the mastery of a modern apparatus of fractal geometry and chaos theory, the ability to develop new and improve existing mathematical methods of analysis, modeling and prediction on the oscillatory fractal geometry and elements of the theory of chaos of the regular and chaotic dynamics (evolution) of complex systems.

The total amount of study time involved in studying discipline is 300 hours for stationer form and 300 hours for the extramural studies.

After mastering this discipline, the postgraduate student must be able to use contemporary or develop new approaches, in particular on the basis of fractal geometry and chaos theory, to analyze, simulate, predict, and program the regular and chaotic dynamics of complex systems from the post-emerging computer experiments.

These methodical instructions are for the second-year PhD students and tests performance in the discipline «Fractal geometry and a Chaos theory».

The main topic Chaotic dynamics of dissipative systems. Elements of the theory of quantum chaos. Chaos in the dynamics of molecular systems in an electromagnetic field.

Methodical instructions for practical work of PhD students, tests performance and distance learning in the discipline «Fractal geometry and a chaos theory», Part 5

Topic: Chaotic dynamics of dissipative systems. Elements of the theory of quantum chaos. Chaos in the dynamics of molecular systems in an electromagnetic field.

Topic: Хаотична динаміка дисипативних систем. Елементи теорії квантового хаосу Хаос в динаміці молекулярних систем в електромагнітному полі. ЗБ- Л4

1. Introduction

To date, the obvious is the fact that the overwhelming number of so -called geophysical, environmental, etc. systems, or, more formally, the systems studied earth sciences are very complex, and this feature is manifested at different spatial and temporal scale levels [1-59]. In this regard, the study of their fundamental properties is still far from satisfactory. As an example of problems whose solution lies in the problems considered in the article, it should be noted the analysis and prediction of the influence of anthropogenic impact on the atmosphere of the industrial city , the development of adequate schemes modeling the properties of the fields of concentration of the air basin industrial city [10]. Naturally, the task list for studying the dynamics of complex systems is not limited to the above examples. It is not difficult to understand that examples of such systems are the atmosphere, turbulent flows in a variety of environments, physical and chemical systems, biological populations, and finally, the society as a communication system and its subsystems: economic, political and other social systems [1-10].

Most important, the fundamental issue in the description of the dynamics of the system is its ability to forecast its future evolution, i.e. predictability of behavior. Recently, the theory of dynamical systems is intensively developed, and, in particular, speech is about the application of methods of the theory to the analysis of complex systems that provide description of their evolutionary dynamics by means solving system of differential equations. If the studied system is more complicated then the greater the equations is necessary for its adequate description. Meanwhile, examples of the systems described by a small

amount of equations, are known nevertheless, theses systems exhibit a complicated behavior. Probably the best-known examples of such systems are the Lorenz system, the Sinai billiard, etc. They are described, for example, three equations (i.e., in consideration included three independent variables), but the dynamics of their behavior over time shows elements of chaos (so-called "deterministic chaos"). In particular, Lorentz was able to identify the cause of the chaotic behavior of the system associated with a difference in the initial conditions. Even microscopic deviation between the two systems at the beginning of the process of evolution leads to an exponential accumulation of errors and, accordingly, their stochastic divergence (as a result, the inability to accurately predict changes in meteorology forecast for a sufficiently long period of time).

During the analysis of the observed dynamics of some characteristic parameters of the systems over time it is difficult to say to what class belongs to the system and what will be its evolution in the future. In recent years for the analysis of time series of fundamental dynamic parameters there are with varying degrees of success developed and implemented a variety of methods, in particular, the nonlinear spectral and trend analysis , the study of Markov chains, wavelet and multifractal analysis, the formalism of the matrix memory and the method of evolution propagators etc. Most of the cited approaches are defined as the methods of a chaos theory. In the theory of dynamical systems methods have been developed that allow for the recording of time series of one of the parameters to recover some dynamic characteristics of the system. In recent years a considerable number of works, including an analysis from the perspective of the theory of dynamical systems and chaos, fractal sets, is devoted to time series analysis of geophysical characteristics, environmental, etc. systems [1-10]. In a series of papers [10-18] the authors have attempted to apply some of these methods in a variety of environmental and hydrodynamic problems. In particular, it is about analyzing and forecasting the anthropogenic impact on the atmosphere of the industrial city. An important result concerning temporal changes in the concentrations of nitrogen dioxide, sulfur dioxide, dust, etc. in the atmosphere of a number of industrial cities, is that the system (atmosphere) exhibits a manifestation of low-dimensional chaos. In connection with this, there is an extremely important task on development of new, more

effective approaches to the nonlinear modeling and prediction of chaotic processes in geophysical and environmental systems.

The essence of new effective approach: Nonlinear modeling of chaotic processes is based on the concept of a compact geometric attractor, which evolve with measurements. We present an advanced approach to analysis and forecasting nonlinear dynamics of chaotic systems, based on conceptions of a chaos methods and neural networks modeling. As example, a few geophysical systems are studied. Since the orbit is continuously rolled on itself due to the action of dissipative forces and the nonlinear part of the dynamics can be found in the neighborhood of any point of the orbit y (n) other points of the orbit yr(n), r = 1, 2, ..., N, that arrive neighborhood y (n) in a completely different times than n. Then you can build different types of interpolation functions that take into account all the neighborhoods of the phase space, and explain how these neighborhoods evolve from y (n) to a whole family of points about y(n+1). Use of the information about the phase space in the simulation of the evolution of the physical process in time can be considered as a major innovation in the modeling of chaotic processes. This concept can be achieved by constructing a parameterized non-linear function F (x, a), which transform y (n) to y(n+1) = F[y(n),a], and then use different criteria for determining the parameters a . Further, since there is the notion of local neighborhoods, we can create a model of the process occurring in the neighborhood, at the neighborhood and by combining together these local models to construct a global non-linear model to describe most of the structure of the attractor. As an illustrative example of using the prediction model, the dynamics of the nitrates concentrations in the Small Carpathians river's watersheds in the Earthen Slovakia during 1969-1996 years is predicted.

2. Method

2.1. Basic idea

The basic idea of the construction of our approach to prediction of chaotic properties of complex systems is in the use of the traditional concept of a compact geometric attractor in which evolves the measurement data, plus the implementation of neural network algorithms. The existing so far in the theory of chaos prediction models are based on the concept of an attractor, and are

described in a number of papers (e.g. [1-10]). The meaning of the concept is in fact a study of the evolution of the attractor in the phase space of the system and, in a sense, modeling ("guessing") time-variable evolution.. From a mathematical point of view, it is a fact that in the phase space of the system an orbit continuously rolled on itself due to the action of dissipative forces and the nonlinear part of the dynamics, so it is possible to stay in the neighborhood of any point of the orbit *y (n)* other points of the orbit y^r *(n), r = 1, 2, ...,* N_B, which come in the neighborhood *y (n)* in a completely different times than *n*. Of course, then one could try to build different types of interpolation functions that take into account all the neighborhoods of the phase space and at the same time explain how the neighborhood evolve from *y (n)* to a whole family of points about *y (n+1)*. Use of the information about the phase space in the simulation of the evolution of some geophysical (environmental, etc.) of the process in time can be regarded as a fundamental element in the simulation of random processes. In terms of the modern theory of neural systems, and neuro-informatics (e.g. [11]), the process of modeling the evolution of the system can be generalized to describe some evolutionary dynamic neuro-equations (miemo-dynamic equations). Imitating the further evolution of a complex system as the evolution of a neural network with the corresponding elements of the self-study, self- adaptation, etc., it becomes possible to significantly improve the prediction of evolutionary dynamics of a chaotic system. Considering the neural network (in this case, the appropriate term "geophysical" neural network) with a certain number of neurons, as usual, we can introduce the operators S_{ij} synaptic neuron to neuron u_i u_j, while the corresponding synaptic matrix is reduced to a numerical matrix strength of synaptic connections: $W = || w_{ij} ||$. The operator is described by the standard activation neuro-equation determining the evolution of a neural network in time:

$$s_i^{'} = sign(\sum_{j=1}^{N} w_{ij} s_j - \theta_i), \qquad (1)$$

where $1< i <N$. Of course, there can be more complicated versions of the equations of evolution of a neural network. Here it is important for us another proven fact related to information behavior neuro-dynamical system. From the point of view of the theory of chaotic dynamical systems, the state of the neuron (the chaos-geometric interpretation of the forces of synaptic interactions, etc.)

can be represented by currents in the phase space of the system and its the topological structure is obviously determined by the number and position of attractors. To determine the asymptotic behavior of the system it becomes crucial information aspect of the problem, namely, the fact of being the initial state to the basin of attraction of a particular attractor. Modeling each geophysical attractor by a record in memory, the process of the evolution of neural network, transition from the initial state to the (following) the final state is a model for the reconstruction of the full record of distorted information, or an associative model of pattern recognition is implemented. The domain of attraction of attractors are separated by separatrices or certain surfaces in the phase space. Their structure, of course, is quite complex, but mimics the chaotic properties of the studied object. Then, as usual, the next step is a natural construction parameterized nonlinear function ***F*** *(x,* ***a****)*, which transforms:

$$\mathbf{y}(n) \rightarrow \quad \mathbf{y}(n+1) = \mathbf{F}(\mathbf{y}(n), \mathbf{a}),$$

and then to use the different (including neural network) criteria for determining the parameters a (see below). The easiest way to implement this program is in considering the original local neighborhood, enter the model(s) of the process occurring in the neighborhood, at the neighborhood and by combining together these local models, designing on a global nonlinear model. The latter describes most of the structure of the attractor.

Although, according to a classical theorem by Kolmogorov-Arnold -Moser, the dynamics evolves in a multidimensional space, the size and the structure of which is predetermined by the initial conditions, this, however, does not indicate a functional choice of model elements in full compliance with the source of random data. One of the most common forms of the local model is the model of the Schreiber type [3] (see also [10]).

2.2. Construction of the model prediction

Nonlinear modeling of chaotic processes is based on the concept of a compact geometric attractor, which evolve with measurements. Since the orbit is continually folded back on itself by the dissipative forces and the non-linear part of the dynamics, some orbit points $\mathbf{y}^r(k)$, $r = 1, 2, \ldots, N_B$ can be found in the

neighbourhood of any orbit point **y**(*k*), at that the points **y**^{r}(*k*) arrive in the neighbourhood of **y**(*k*) at quite different times than *k*. Then one could build the different types of interpolation functions that take into account all the neighborhoods of the phase space, and explain how these neighborhoods evolve from y (n) to a whole family of points about y (n + 1). Use of the information about the phase space in modeling the evolution of the physical process in time can be regarded as a major innovation in the modeling of chaotic processes.

This concept can be achieved by constructing a parameterized nonlinear function F (x, a), which transform y (n) to y (n + 1) = F (y (n), a), and then using different criteria for determining the parameters a. Further, since there is the notion of local neighborhoods, one could create a model of the process occurring in the neighborhood, at the neighborhood and by combining together these local models to construct a global nonlinear model that describes most of the structure of the attractor.

Indeed, in some ways the most important deviation from the linear model is to realize that the dynamics evolve in a multidimensional space, the size and the structure of which is dictated by the data. However, the data do not provide "hints" as to which model to select the source to match the random data. And the most simple polynomial models, and a very complex integrated models can lead to the asymptotic time orbits of strange attractors, so for part of the simulation is connected with physics. Therefore, physics is "reduced" to fit the algorithmic data without any interpretation of the data. There is an opinion that there is no algorithmic solutions on how to choose a model for a mere data.

As shown Schreiber [3], the most common form of the local model is very simple :

$$s(n+\Delta n) = a_0^{(n)} + \sum_{j=1}^{d_A} a_j^{(n)} s(n-(j-1)\tau) \qquad (2)$$

where Δ n - the time period for which a forecast . The coefficients $a_j^{(k)}$, may be determined by a least-squares procedure, involving only points *s*(*k*) within a small neighbourhood around the reference point. Thus, the coefficients will vary throughout phase space. The fit procedure amounts to solving (d_A + 1) linear equations for the (d_A + 1) unknowns. When fitting the parameters *a*, several problems are encountered that seem purely technical in the first place but are related to the nonlinear properties of the system. If the system is low-

dimensional, the data that can be used for fitting will locally not span all the available dimensions but only a subspace, typically. Therefore, the linear system of equations to be solved for the fit will be ill conditioned. However, in the presence of noise the equations are not formally ill-conditioned but still the part of the solution that relates the noise directions to the future point is meaningless . Note that the method presented here is not only because, as noted above, the choice of fitting requires no knowledge of physics of the process itself. Other modeling techniques are described, for example, in [3,10].

Assume the functional form of the display is selected, wherein the polynomials used or other basic functions. Now, we define a characteristic which is a measure of the quality of the curve fit to the data and determines how accurately match y (k + 1) with F (y (k), a), calling it by a local deterministic error:

$$\varepsilon_D(k) = \mathbf{y}(k+1) - \mathbf{F}(\mathbf{y}(k), \mathbf{a}). \qquad (3)$$

The cost function for this error is called W (ε). If the mapping F (y, a), constructed by us, is local, then one has for each adjacent to y (k) point, y $^{(r)}$ (k) (r = 1, 2, ..., N_B),

$$\varepsilon_D^{(r)}(k) = \mathbf{y}(r, k+1) - \mathbf{F}(\mathbf{y}^{(r)}(k), \mathbf{a}), \qquad (4)$$

where y (r, k + 1) - a point in the phase space which evolves y (r, k). To measure the quality of the curve fit to the data, the local cost function is given by

$$W(\varepsilon, k) = \frac{\sum_{r=1}^{N_B} \left|\varepsilon_D^{(r)}(k)\right|^2}{\sum_{r=1}^{N_B} \left[\mathbf{y}(k) - \langle \mathbf{y}(r,k) \rangle\right]^2} \qquad (5)$$

and the parameters identified by minimizing W (ε, k), will depend on a.

Furthermore, formally the neural network algorithm is launched, in particular, in order to make training the neural network system equivalent to the reconstruction and interim forecast the state of the neural network (respectively, adjusting the values of the coefficients). The starting point is a formal knowledge of the time series of the main dynamic parameters of a chaotic system, and then to identify the state vector of the matrix of synaptic interactions | | w_{ij} | | etc. Of course, the main difficulty here lies in the implementation of the

process of learning neural network to simulate the complete process of change in the topological structure of the phase space of the system and use the output results of the neural network to adjust the coefficients of the function display. The complexity of the local task, but obviously much less than the complexity of predicting the original chaotic processes in geophysical or other dynamic systems .

2. 3. The illustrative example: polarization time series for molecular systems in electromagnetic field

The typical theoretical time dependence of polarization for ZrO molecule in the field in a chaotic regime is presented in Figure 1.

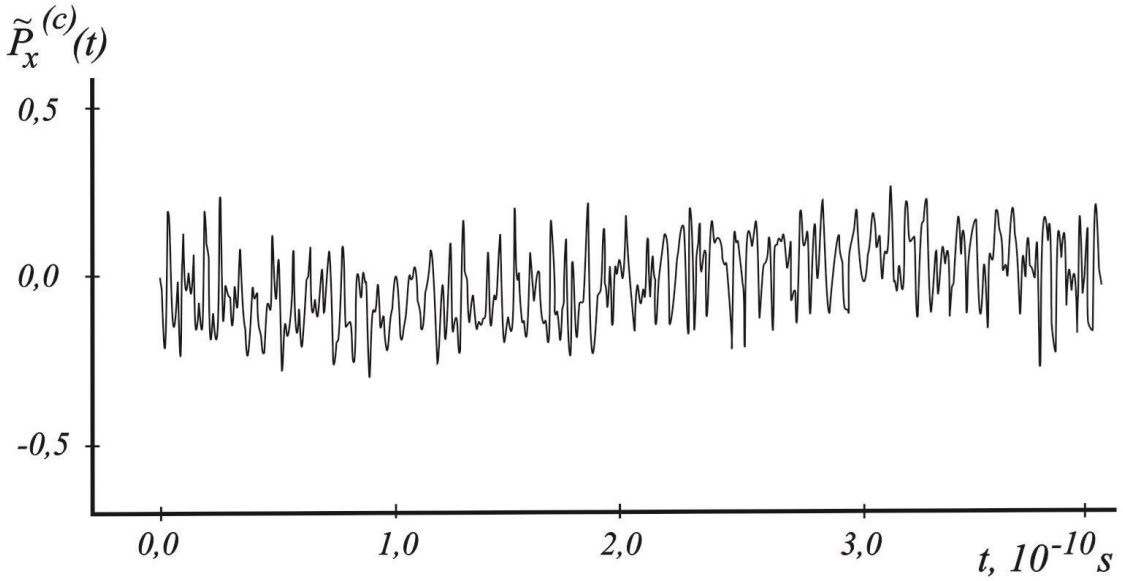

Figure 1. The typical theoretical time-dependence of polarization *p(t)* of the ZrO molecule in a linearly polarized field (see parameters in text).

The polarization is normalized to the intensity of the field interaction with the molecule. The next step is application of the chaos-geometric approach to analysis of the temporal 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 3 we list the computed values of the correlation dimension d_2, the Kaplan-York attractor dimension (d_L), the Lyapunov's exponents (λ_i, i=1-3), the Kolmogorov entropy (K_{entr}), and the Gottwald-Melbourne parameter.

Table 3. The correlation dimension d_2, Lyapunov's exponents (λ_i, i=1,2), Kaplan-York attractor dimension (d_L), Kolmogorov entropy (K_{entr}), the Gottwald-Melbourne parameter K_{GW}

Molecule	d_2	λ_1	λ_2	d_L	K_{entr}	K_{GW}
ZrO	2.76	0.147	0.018	2.53	0.165	0.73

Analysis of the presented data allows to make conclusions that the dynamics of the ZrO molecule in a resonant linearly polarized electromagnetic field has the elements of a deterministic chaos (the strange attractor) and this conclusion is entirely agreed with the results of modelling for other diatomic molecules [17-22].

As example of using an approach to predict the polarization time dependence (see above), in Figure 2 we present the original theoretical (solid line) and predicted (dotted line) lines of polarization $p(t)$ for the ZrO molecule in a linearly polarized field (one thousand twenty points).

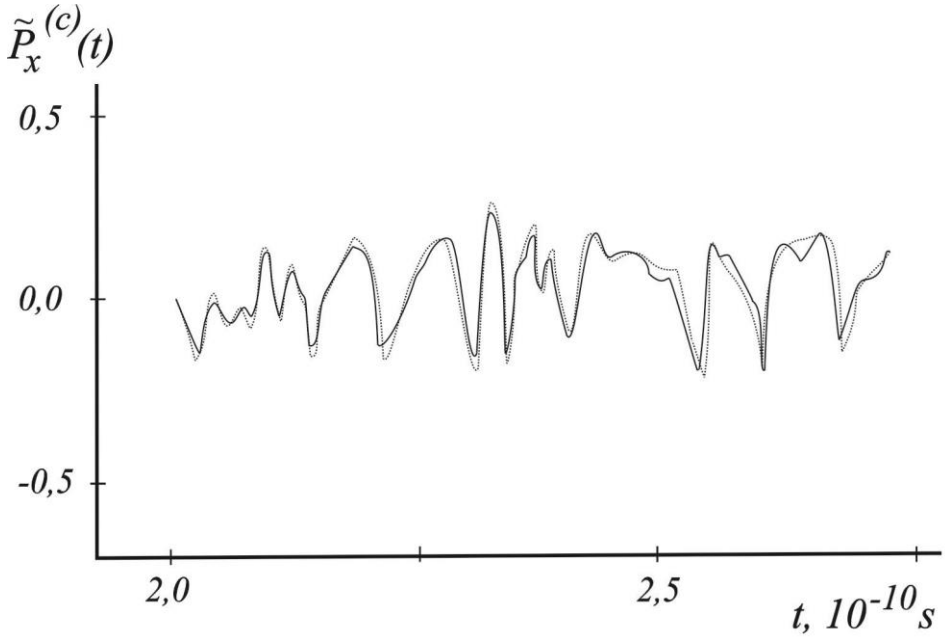

Figure 2. The original theoretical (solid line) and predicted (dotted line) time dependence lines of polarization $_{p(t)}$ of the ZrO molecule in a linearly polarized field.

Despite some difference between the forecast and the actual data, in any case the presented results can be considered quite satisfactory.

3. Tests performance

Test Option 1.

1). Give the key definitions of united conceptions of a chaos methods and neural networks modeling in dynamics of classical and quantum systems on example of the molecular systems in the resonant electromagnetic field: i) mathematical and physical essense, ii) united conceptions of a chaos methods and neural networks modeling , iii) spectral statistics on molecular parameters, iv) definitions of a chaos topological and dynamical invariants. V). forecasing of the polarization tine series

2). Explain all definitions om the example of the concrete quantum system: **molecule of NdO** preliminarily describing the corresponding features of spectrum of a molecule from pointwiew of fractal geometry and a chaos theory.

3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule” for the atom from the first task of the option (all necessary numerical parameters should be self-taken) and calculate a chaos phenomenon topological and dynamical invariants for the corresponding molecular system in a field. Provide forecasing of the polarization tine series of the **NdO.**

Test Option 2.

1). Give the key definitions of united conceptions of a chaos methods and neural networks modeling in dynamics of classical and quantum systems on example of the molecular systems in the resonant electromagnetic field: i) mathematical and physical essense, ii) united conceptions of a chaos methods and neural networks modeling , iii) spectral statistics on molecular parameters, iv) definitions of a chaos topological and dynamical invariants. V). forecasing of the polarization tine series

2). Explain all definitions om the example of the concrete quantum system: **molecule of CeO** preliminarily describing the corresponding features of spectrum of a molecule from pointwiew of fractal geometry and a chaos theory.

3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule” for the atom from the first task of the option (all necessary numerical parameters should be self-taken) and calculate a chaos phenomenon topological and dynamical invariants for the corresponding molecular system in a field. Provide forecasing of the polarization tine series of the Ce**O.**

Test Option 3.

1). Give the key definitions of united conceptions of a chaos methods and neural networks modeling in dynamics of classical and quantum systems on example of the molecular systems in the resonant electromagnetic field: i) mathematical and physical essense, ii) united conceptions of a chaos methods and neural networks modeling , iii) spectral statistics on molecular parameters, iv) definitions of a chaos topological and dynamical invariants. V). forecasing of the polarization tine series

2). Explain all definitions om the example of the concrete quantum system: **molecule of ZrO** preliminarily describing the corresponding features of spectrum of a molecule from pointwiew of fractal geometry and a chaos theory.

3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule” for the atom from the first task of the option (all necessary numerical parameters should be self-taken) and calculate a chaos phenomenon topological and dynamical invariants for the corresponding molecular system in a field. Provide forecasing of the polarization tine series of the **ErO.**

Test Option 4.

1). Give the key definitions of united conceptions of a chaos methods and neural networks modeling in dynamics of classical and quantum systems on example of the molecular systems in the resonant electromagnetic field: i) mathematical and physical essense, ii) united conceptions of a chaos methods and neural networks modeling , iii) spectral statistics on molecular parameters, iv) definitions of a chaos topological and dynamical invariants. V). forecasing of the polarization tine series

2). Explain all definitions om the example of the concrete quantum system: **molecule of CeO** preliminarily describing the corresponding features of spectrum of a molecule from pointwiew of fractal geometry and a chaos theory.

3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule” for the atom from the first task of the option (all necessary numerical parameters should be self-taken) and calculate a chaos phenomenon topological and dynamical invariants for the corresponding molecular system in a field. Provide forecasing of the polarization tine series of the **ErO.**

Test Option 5.

1). Give the key definitions of united conceptions of a chaos methods and neural networks modeling in dynamics of classical and quantum systems on example of the molecular systems in the resonant electromagnetic field: i) mathematical and physical essense, ii) united conceptions of a chaos methods and neural networks modeling , iii) spectral statistics on molecular parameters, iv) definitions of a chaos topological and dynamical invariants. V). forecasing of the polarization tine series

2). Explain all definitions om the example of the concrete quantum system: **molecule of GdO** preliminarily describing the corresponding features of spectrum of a molecule from pointwiew of fractal geometry and a chaos theory.

3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule” for the atom from the first task of the option (all necessary numerical parameters should be self-taken) and calculate a chaos phenomenon topological and dynamical invariants for the corresponding molecular system in a field. Provide forecasing of the polarization tine series of the **GdO.**

Test Option 6.

1). Give the key definitions of united conceptions of a chaos methods and neural networks modeling in dynamics of classical and quantum systems on example of the molecular systems in the resonant electromagnetic field: i) mathematical and physical essense, ii) united conceptions of a chaos methods and neural networks modeling , iii) spectral statistics on molecular parameters, iv) definitions of a chaos topological and dynamical invariants. V). forecasing of the polarization tine series

2). Explain all definitions om the example of the concrete quantum system: **molecule of PmO** preliminarily describing the corresponding features of spectrum of a molecule from pointwiew of fractal geometry and a chaos theory.

3). To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Supermolecule” for the atom from the first task of the option (all necessary numerical parameters should be self-taken) and calculate a chaos phenomenon topological and dynamical invariants for the corresponding molecular system in a field. Provide forecasing of the polarization tine series of the Pm**O.**

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