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Nonlinear Dynamics of Molecular Systems in an External Electromagnetic Field: Classical and Quantum Treatment of Chaos and Strange Attractors

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Abstract: An effective computational approach to studying nonlinear chaotic dynamics of the diatomic and multiatomic molecules) including complex spectra, deterministic chaos, strange attractors) in an external infrared electromagnetic field is presented. The approach includes combined quantum-mechanical model (based on the solution of the molecular Schrödinger equation, and realistic model potential method and advanced dynamical systems and nonlinear analysis methods such as a spectral and multifractal algorithm, analysis on the basis of the Lyapunov's exponents and the Kolmogorov entropy etc. The polarization time series for a molecule in an infrared field are analyzed and computed. The results of computing the dynamical and topological invariants for dynamics of a number of the diatomic molecules (GeO, ZrO, PbO and others) in the infrared electromagnetic field with intensity of 25 GW/cm^2 are presented. The principally new result is in development of an effective non-linear prediction model for the polarization time series. It is shown that even though the simple procedure is used to construct the non-linear model, the predicted results for the polarization time series of the studied molecules are quite satisfactory.

Keywords: dynamics of atomic systems, spectral features, chaos and attractors

1. Introduction. Nonlinear Dynamics of Molecular Systems in Electromagnetic Field

At present time it is of a great interest a study of phenomenon of quantum chaos in complex molecular systems. This interest is provided by a whole number of important scientific and technical applications, including a necessity of understanding chaotic features in a work of different electronic devices and systems. New field of investigations of the nonlinear chaotic dynamics of molecular systems in an electromagnetic field has been provided by a great progress in a development of effective quantum mechanical methods as well as the further progressing a chaos theory and dynamic systems methods and algorithms. For example, a transition from regular motion to dynamical chaos for a diatomic molecule in a linearly (or circularly) polarized resonant electromagnetic field is connected with the overlapping of vibrational-rotational nonlinear resonances [1,2]. Studying the chaotic dynamics of molecular systems has shown that a chaos phenomenon may significantly affect the intramolecular vibrational energy redistribution, assigning the vibrational spectra, coherent control of the intramolecular processes and a dynamics of molecules interacting with a resonant electromagnetic field etc [2-4]. In this paper we present an effective computational approach to studying nonlinear chaotic dynamics of the diatomic and multiatomic molecules) including complex spectra, deterministic chaos, strange attractors) in an external infrared electromagnetic field is presented. The approach

includes combined quantum-mechanical model (based on the solution of the molecular Schrödinger equation, and realistic model potential method) and advanced dynamical systems and non-linear analysis methods such as a non-linear analysis methods including correlation (dimension D) integral, fractal analysis, average mutual information, false nearest neighbours, Lyapunov's exponents and Kolmogorov energy analysis, power spectrum and surrogate data algorithms, stochastic propagators method, memory and Green's functions approaches etc methods etc.

2. Model, Results and Concluding Remarks

A chaotic dynamics analysis for diatomic molecules in an intense electromagnetic field) is based on the numerical solution of the time-dependent Schrödinger equation and realistic model potential approximation $U(x)$ and, secondly, using the universal chaos -geometric approach to analysis of nonlinear chaotic dynamics (chaos-geometric unit). The problem is reduced to solving the Schrödinger equation [2,3]:

$$i\partial\Psi/\partial t = [H_0 + U(x) - d(x)E_M\varepsilon(t)\cos(\omega_L t)]\Psi \quad (1)$$

where E_M - the maximum field strength, $\varepsilon(t)=E_0\cos(\nu t)$ corresponds the pulse envelope. Molecule in the field gets induced polarization and its high-frequency component can be defined as [6]:

$$p_c^{(x,y)}(t) = \left(\frac{1}{T}\right)\oint\langle\psi(t)|\hat{d}_{x,y}|\psi(t)\rangle\cos\omega t dt, \quad (2)$$

where T — period of the external field, d –dipole moment.

The test numerical computing the dynamics of the diatomic molecule GeO in the linearly polarized field (molecule and field parameters are as : $\hbar\Omega$=985.8 cm^{-1}, $y\hbar\Omega$=4.2cm^{-1}, B = 0.48 cm^{-1}, d_0 = 3.28 D, M=13.1 a.e.м.; the intensity 2.5-25 GW/cm^2, respectively: W = 3.39-10.72 cm^{-1}) has been carried out and copared with earlier obtaimed results. According to classical-dynamical treating these parameters correspond to chaotic regime. The analysis shows that more than 200 vibrational-rotational molecular levels are involved into a chaotic dynamics. There are presented the calculated quantitative parameters for the GeO molecule chaotic dynamics in a linearly polarized field of the intensity 25 GW / cm^2, namely, dynamical and topological invariants: correlation dimension (2.73), the embedding dimension (3), Kaplan-Yorke dimension (2.51), LE (first two LE are positive: + 0.146 + 0.0179), Kolmogorov entropy (0.16) and others. The analogous data are listed for other studied molecules (PbO, ZrO etc).

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