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Chaotic dynamics of diatomic systems in an electromagnetic field: Dynamical and topological invariants

An advanced combined quantum-dynamic and chaos-geometric method for analysis, modelling, and forecasting of the chaotic dynamics of diatomic molecules in an intense electromagnetic field is presented. The method is based on the use of the non-stationary theory of the Schrödinger equation in the approximation of the density functional and the methods of the theory of chaos and dynamic systems for the analysis of time series of polarization and other characteristics of diatomic molecules in an intense electromagnetic field. In particular, the latter includes the Gottwald-Melbourne test, the correlation integral method , fractal and multifractal formalism, average mutual information, false nearest neighbours, surrogate data algorithms, analysis on the basis of the Lyapunov's exponents, Kolmogorov entropy, nonlinear forecast models based on algorithms of optimized predicted trajectories, B-spline approximations. As an illustration, the advanced data for the dynamical and topological invariants (correlation dimension, embedding dimension, Kaplan-York dimension, Lyapunov's exponents, Kolmogorov entropy, etc.) for the diatomic ZrO molecule in a linearly polarized electromagnetic field are listed.

***Key words**: diatomic systems in an electromagnetic field, chaotic dynamics, chaos-geometric approach, dynamical and topological invariants*

Introduction. Currently, the theoretical and experimental study of regular and chaotic dynamics of nonlinear processes in various classes of quantum systems (in particular, atomic and molecular systems in an external electromagnetic field) is of great interest, which is of great importance to many scientific and technical applications, etc. [1-10]. Chaos theory establishes that apparently complex irregular behaviour can be the result of a simple deterministic system with several dominant nonlinear interdependent variables. A large number of studies using ideas derived from chaos science to characterize, model, and predict the dynamics of various system phenomena have been witnessed over the last decade (see, for example, [11–23]). The results of such studies are very encouraging, as they not only showed that the dynamics of clearly irregular phenomena can be understood from a chaotic deterministic point of view, but also reported very good predictions using this approach for various systems, including those that from a classical point of view were considered non-prognostic. This is a well-known problem of modern chaos theory and dynamical systems. We should mention the interpretation of chaotic phenomena in quantum systems through the mechanism of strong nonlinear interaction and overlap of resonances (overlapping and merging resonances, "snapshots" of gas resonances, stochastization of oscillatory motion in molecules, etc). A well-known example of complex nonlinear chaotic dynamics of finite quantum systems is the chaotic dynamics of a hydrogen atom or Rydberg atoms or more complex molecular systems in an external electromagnetic field (see [1-4, 23-26]).

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In this article, we present the results of applying the combined quantum-dynamic and chaos-geometric method [27-30] for analysis, modelling, and forecasting of the chaotic dynamics of diatomic molecules in an intense electromagnetic field and list the advanced data for dynamical and topological invariants, characterizing the polarization time series for the diatomic ZrO molecule in a linearly polarized electromagnetic field of high intensity.

Theoretical method. Our approach to modeling the chaotic dynamics of diatomic molecules in an intense electromagnetic field is based on two blocks, namely, the universal nonlinear analysis block (e.g.[18-23]), which in our problem actually includes the computation of time series of level populations, polarization, power spectrum, and quantum-dynamic block (e.g. [27-30]). The latter includes solutions of the time-dependent Schrödinger equation for the diatomic molecule in an electromagnetic field, computing the molecule polarization and other parameters. The chaotic behavior could be identified using the Lyapunov's exponent, the separation of two adjacent trajectories, and the Fourier transform of the temporal evolution of the system.

As the applied method has been earlier in details presented in refs. [18-23, 27-30], including the quantum-dynamic method of description of the diatomic molecule in an electromagnetic field, below we will restrict yourself only by some fundamental definitions and key ideas. The quantum-dynamic approach to a diatomic molecule in an electromagnetic field is based on the solution of the time-dependent Schrödinger equation, optimized operator perturbation theory and realistic interatomic potential. For the studied molecule we have used the results of computing in the density functional approximation (e.g. [29,30]). A molecule in the field gets the induced polarization and its high-frequency component can be determined and listed as the corresponding time series [28,30]. It is well known that a spectrum in the regular case of molecular dynamics consists of a little quantity of the well resolved lines. Principally another physical and mathematical situation occurs in the case of chaotic dynamics of molecule in a field. It is easily to understand [30] that the corresponding energy of interaction with an electromagnetic field can be much higher than the known anharmonicity constant, i.e., $W > xh\Omega$, and, as result, the corresponding spectrum in this case becomes significantly more complicated [27, 30].

The main output data of the quantum-dynamical modelling are the corresponding time series for the polarization of a molecule in a resonant electromagnetic field in a chaotic regime (e.g., [30]). In order to perform the detailed analysis of the chaotic dynamics of the molecule in an electromagnetic field through mathematical analysis of the corresponding polarization time series, and to compute the well-known fundamental topological and dynamical invariants of the system in a chaotic regime the universal chaos-geometric approach (e.g.[18-23,27-30]) has been used, in particular, the version [28,30].

In general, the chaos-geometric approach includes using a combined set of such non-linear analysis, dynamical systems and a chaos theory methods as the Gottwald-Melbourne test, the correlation integral method, algorithms of average mutual information, false nearest neighbors, surrogate data, methods of analysis based on the

Lyapunov's exponents, Kolmogorov entropy, power spectrum, nonlinear prediction models, based on algorithms of optimized predicted trajectories, B-spline approximations, neural network simulation algorithms etc (e.g.[11-18,27-30]).

It is worth to remind that the master task of mathematical modeling molecular parameter time series for analysis of dynamics of diatomic molecule in a field here is to determine the corresponding embedding dimension and to reconstruct a Euclidean space R^d large enough so that the set of points d_A can be unfolded without ambiguity [12,14,18,29]. In accordance with the embedding theorem, the embedding dimension, d_E, must be greater, or at least equal, than a dimension of attractor, d_A, i.e. $d_E > d_A$.

In order to reconstruct the corresponding attractor dimension (e.g., [12-15,18]) one could use two main standard approaches. The first approach is the well-known correlation integral analysis (e.g. [15]), which is one of the widely used techniques to investigate the signatures of chaos in a time series. The method introduces the correlation integral, $C(r)$, to distinguish between chaotic and stochastic systems. To compute the correlation integral, the standard algorithm by Grassberger-Procaccia [15] is usually used. The problem is reduced to computing the next quantity:

$$C(r) = \lim_{N\to\infty} \frac{2}{N(n-1)} \sum_{\substack{i,j \\ (1\le i<j\le N)}} H\left(r - \| y_i - y_j \|\right), \qquad (1)$$

where H is the Heaviside step function with $H(u) = 1$ for $u > 0$ and $H(u) = 0$ for $u \le 0$, r is the radius of sphere centered on $\mathbf{y}_i$ or $\mathbf{y}_j$, and N is the number of data measurements. In order to provide the strict verification of the correlation integral algorithm analysis results, it is additionally useful to apply another method, which is called as the surrogate data method [14, 18]. This approach makes use of the surrogate data, generated in accordance to the probabilistic structure underlying the original data. Here we have used the version [18, 28].

One the most important dynamical invariants of a chaotic system are the well-known Lyapunov's exponents (e.g., [14-17]). Usually these invariants are determined as asymptotic average rates. The Lyapunov's exponents are independent of the initial conditions, and do comprise an invariant measure of attractor. Usually, the computing of the Lyapunov's exponents allows quickly determine whether the system is chaotic or not. Another master invariant is the Kolmogorov entropy K_{ent} , which, according to definition, measures the average rate at which information about the state is lost with time. Numerically, the Kolmogorov entropy can be determined as the sum of the positive Lyapunov's exponents. The estimate of the dimension of the attractor is provided by the Kaplan and York conjecture:

$$d_L = j + \frac{\sum_{a=1}^{j} \lambda_a}{\left|\lambda_{j+1}\right|}, \qquad (2)$$

where j is such that $\sum_{a=1}^{j} \lambda_a > 0$ and $\sum_{a=1}^{j+1} \lambda_a < 0$, and the Lyapunov's exponents λ_a are taken in descending order. The detailed information about the cited characteristics as well as the details of the main computational algorithms to determine the topological and dynamical invariants can be found in Refs. [11-18, 27-30]).

Some results and conclusion. Below there are listed the results of computational analysis of the time dynamics for diatomic molecule ZrO in the electromagnetic field. According to [25], the parameter W of interaction of an electromagnetic radiation with a molecule is as follows:

$$W\left[\text{cm}^{-1}\right] = 120.3\left(d_0/r_0\right)\left(S/M\omega_e\right)^{1/2} \quad (3)$$

where, as usually, an electromagnetic field is standardly characterized by the following parameter: $S = cE/8\pi$ (c is the velocity of light and E is a field strength), an interatomic distance r_0 in Å, dipole moment d_o in D, ω_e in cm^{-1}, M in a.u.m., and the field parameter S in GW/cm^2. The set of the ZrO molecular constants and electromagnetic field parameters is listed in Table 1 [28,31,32].

It is easily to find that the known Chirikov chaotic parameter in our case is as follows:

$$\delta n = 2\left(Ed/B\right)^{1/2} \gg 1. \quad (4)$$

The typical theoretical time dependence of polarization for ZrO molecule in the field in a chaotic regime is presented in Ref. [28]. The number of the points and the concrete time step in analyzing the corresponding time series of polarization are as follows: $n = 7.6\cdot10^3$ and $\Delta t = 5\cdot10^{-14}$ s. In Table 2 there are listed the computational data for the correlation dimension d_2, the Kaplan-York attractor dimension (d_L), the Lyapunov's exponents (λ_a), Kolmogorov entropy (K_{entr}), the Gottwald-Melbourne parameter K_{GW}.

From table one could see that the first two Lyapunov's exponents are positive. In whole, the data on dynamical and topological parameters demonstrate the availa-

Table 1. Set of the ZrO molecular constants and electromagnetic field parameters

Parameters	PbO
$\omega_e = \hbar\Omega$ (cm^{-1})	969.7
$\omega_e x_e = x\hbar\Omega$ (cm^{-1})	6.90
B_e (cm^{-1})	0.423
D_e (cm^{-1})	$3.19\text{x}10^{-7}$
d_0 (D)	2.55
r_0 (Å)	1.72
M (a.u.m)	13.58
W (cm^{-1})	15.5-49.1

Table 2. Correlation dimension d_2, the Lyapunov's exponents (λ_i, i=1,2), the Kaplan-York attractor dimension (d_L), the 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

bility of the dynamical chaos elements (indeed the low-dimensional attractor) in behavior of diatomic molecule ZrO, interacting with electromagnetic field.

To conclude, an advanced version of the quantum-dynamic and chaos-geometric method is adapted for modelling the chaotic dynamics of diatomic molecules in an intense electromagnetic field, which is based on the theory of the time-dependent Schrödinger equation and the apparatus for modelling, analysis, forecasting time series of polarization and other characteristics of molecules using such chaos theory methods as the Gottwald-Melbourne test, the correlation integral method, the algorithms of average mutual information, false nearest neighbors, surrogate data, methods of analysis based on the Lyapunov's exponents, Kolmogorov entropy, etc.

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Г.В. Ігнатенко, Т.Б. Ткач, І.В. Іванова

Хаотична динаміка двоатомних систем в електромагнітному полі: Динамічні та топологічні інваріанти

АНОТАЦІЯ

Представлено удосконалений комбінований квантово-динамічний та хаос-геометричний метод до аналізу, моделювання, прогнозування хаотичної динаміки двоатомних молекул в інтенсивному електромагніт-ному полі. Метод базується на використанні нестаціонарної теорії рівняння Шредінгеру в наближенні функціоналу густини і методів теорії хаосу та динамічних систем для аналізу часових рядів поляризаційних та інших характеристик двоатомних молекул в інтенсивному електромагніт-ному полі. Методи теорії хаосу та систем включать, зокрема, тест Gottwald-Melbourne, метод кореляційного інтегралу, мультіфрактальний формалізм, алгоритми середньої взаємної інформації, хибних найближчих сусідів, сурогатних даних, методи аналізу на основі показників Ляпунова, ентропії Колмогорова, моделі нелінійного прогнозу на основі алгоритмів оптимізованих передбачених траєкторій, B-сплайнових апроксимації та нейромережевих алгоритмів тощо. В якості ілюстрації наведені дані обчислень динамічних і топологічних інваріантів (кореляційна розмірність, розмірність вкладення, розмірність Каплана-Йорка, показники Ляпунова, ентропія Колмогорова і т.і.) для двохатомної молекули ZrO в лінійно поляризованому електромагнітному полі високої інтенсивності.

Ключові слова: *двоатомні системи в електромагнітному полі, хаотична динаміка, хаос-геометричний підхід, динамічні та топологічні інваріанти*