UDC 539.184, 539.186

A. V. Ignatenko, A. A. Kuznetsova, A. S. Kvasikova, A. V. Glushkov, M. Yu. Gurskaya

Odessa State Environmental University, 15, Lvovskaya str., Odessa, Ukraine
Odessa National Maritime Academy, Odessa, 4, Didrikhsona str., Odessa, Ukraine
Odessa National Polytechnical University, 1, Shevchenko av., Odessa, Ukraine
e-mail: quantign@mail.ru

NONLINEAR CHAOTIC DYNAMICS OF ATOMIC AND MOLECULAR SYSTEMS IN AN ELECTROMAGNETIC FIELD

It has been numerically studied a chaotic dynamics of diatomic molecules (on example of the GeO molecule in an infrared field) and some laser systems. An advanced generalized techniques such as the wavelet analysis, multi-fractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, the Lyapunov exponent's (LE) analysis, and surrogate data method, prediction models etc is used. It has been shown that systems exhibit a nonlinear behaviour with elements of a low-or high-dimensional chaos. There are firstly presented the numerical data on topological and dynamical invariants of chaotic systems, in particular, the correlation, embedding, Kaplan-York dimensions, LE, Kolmogorov's entropy etc for GeO molecule in an electromagnetic infrared field in the chaotic regime..

In last years the phenomena of dynamical chaos and dynamical stabilization attract a great interest as a manifestation of this effect in photo-optical systems may in a significant degree change a functional regime (e.g.[1-15]). Cited effect is usually observed in the physical systems and related to a type of non-linear effects. As a rule, dynamical chaos is manifested in the quantum systems, which are not linear in a classic limit. Above especially effective manifestations of this effect in the quantum systems one could mention systems which interact with external, time dependent, for example laser, field. It has been discovered that dynamics of atomic and molecular, cluster and nano-optical systems in a laser field has features of the random, stochastic kind and its realization does not require the specific conditions. The importance of studying a phenomenon of stochasticity or quantum chaos in dynamical systems in laser field is provided by a whole number of technical applications, including a necessity of understanding chaotic features in a work of different electronic devices and systems. The important topic of the laser-atomic dynamics and hierarchy systems physics is connected with governing and control of quantum chaotic diffusion and stabilisation effects in atomic systems in the intense laser field (especially important case is atoms in electromagnetic traps and heat bath) [2,15,16]. The principal aim of coherent control is to steer a quantum system towards a desired final state through interaction with light while simultaneously inhibiting paths leading to undesirable outcomes. Controlling mechanisms have been proposed and demonstrated for atomic and solid-state systems. Gibson performs calculations for three-level systems and 1D model of a two-electron molecule (see refs in [3]). Transitions to excited state occur via a 12-photon interaction for an 800 nm intense pulse of length 244 au, or just over 2 cycles. The stabilization dynamics of model He beyond the dipole approximation and with two active electrons was is investigated [6] in the presence of a high-intensity and high-frequency laser pulse. There may exist a laser frequency and intensity regime in which the total ionization yield decreases with increasing laser amplitude. In the near future, free electron lasers will further deliver laser pulses of such high frequencies and intensities to meet the conditions needed for the stabilization of atomic systems more easily. Along with those technological de-

velopments, a wide range of theoretical methods including analytical model calculations, Monte Carlo simulations and numerical calculations have been applied to the ionization of hydrogen-like atoms. Further progress was achieved concerning the ionization and stabilization of atoms with two active electrons. In ref.[11,12] an effective approach to adequate treating and sensing a spectral hierarchy and dynamical stabilisation in atomic systems in the intense laser field is considered and based on non-relativistic and relativistic time-dependent complex rotation method (for atomic systems) and non-Hermitian Floquet formalism (for molecular systems). The stabilization of helium (study of the 2D two-electron atom) in intense high-frequency laser pulses is modelled within the relativistic scheme. It has been carried out modeling generation of the atto-second VUV and X-ray pulses under ionization of atomic (molecular) system by femto-second optical pulse.

In this paper we present the results of analysis of the chaotic dynamics for diatomic molecules in an electromagnetic (infrared) field. In this paper we numerically studied a chaotic dynamics of diatomic molecules (on example of the GeO molecule in an infrared field) and some laser systems.

An advanced generalized techniques such as the wavelet analysis, multi-fractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, the Lyapunov exponent's (LE) analysis, and surrogate data method, prediction models etc (look details in Refs.[3-19]) is used. It has been shown that systems exhibit a nonlinear behaviour with elements of a low-or high-dimensional chaos. There are firstly presented the numerical data on topological and dynamical invariants of chaotic systems, in particular, the correlation, embedding, Kaplan-York dimensions, LE, Kolmogorov's entropy etc for GeO molecule in an electromagnetic infrared field in the chaotic regime.

The analysis is based on the numerical solution of the time-dependent Schrödinger equation and realistic Simons-Parr-Finlan model for the potential of diatomic molecule $U(x)$ (the quantum unit). Secondly, it is based on using an universal approach to analysis of nonlinear chaotic dynamics (chaos-geometric unit). The Simons-Parr-Finlan formulae [20] for the molecular potential is:

$$U(r) = B_0[r - r_e)/r]^2\{1 + \sum_n b_n[r - r_e)/r]^n\} \quad (1a)$$

or introducing $x = r - r_0$:

$$U(r) = B_0[x(x + r_0]^2\{1 + \sum_n b_n[x(x + r_0]^n\} \quad (1b)$$

where the coefficients b_i are linked with corresponding molecular constants [20].

The problem of dynamics of diatomic molecules in an infrared field is reduced to solving the Schrödinger equation:

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

where E_M - the maximum field strength, $e(t)=E_0 cos(nt)$ corresponds the pulse envelope (chosen equal to one at the maximum value of electric field). A molecule in the field gets the induced polarization and its high-frequency component can be defined as:

$$P_x(t) = p_c^{(x)}(t)cos\omega t + p_s^{(x)}(t)sin\omega t,$$
$$P_y(t) = p_c^{(y)}(t)cos\omega t + p_s^{(y)}(t)sin\omega t,$$
$$p_c^{(x,y)}(t) = \left(\frac{1}{T}\right)\oint\langle\psi(t)|\hat{d}_{x,y}|\psi(t)\rangle cos\omega t dt, \quad (3)$$

where T – period of the external field, d –dipole moment. The power spectrum can be further determined as $S(\omega) = |F[p(t)]|^2$. To avoid the numerical noise during the Fourier transformation, the attenuation technique used,i.e. at $t > t_p$, p (t) is replaced by

$$p(t)cos^2\{\pi(t - t_p)/[2(T - t_p)]\}, \quad (t_p < t < T)$$
with $T=1.6t_p$. (4)

It is understood that in the regular case of molecular dynamics, a spectrum will consist of a small number of the well resolved lines. In the case of chaotic dynamics of molecule in a field situation changes essentially. The corresponding energy of interaction with the field is much higher than anharmonicity constant $W > x\hbar\Omega$. It is obvious that a spectrum in this case become more complicated [17,18].

We have carried out the numerical computing dynamics of the diatomic molecule GeO in the electromagnetic field (the molecule and field parameters are as follows : $\hbar\Omega$=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 field intensity is 2.5-25 GW/cm^2, respectively: W = 3.39-10.72cm^{-1}). The corresponding Chirikov parameter in this case is as: $\delta n = 2(Ed/B)^{\frac{1}{2}} \gg 1$.

According to classical-dynamical treating [41], these parameters correspond to chaotic regime. The principle of quantum mechanics enter, of course, into the mixed interpretation in terms of classical trajectories [42]. From one side, the final answers are at least understandable intuitively, from other one they are result of numerical analysis of complex molecular dynamics, which involve a superposition of high-order energy transitions, intensive interaction of non-linear resonances and chaotic motion of a molecule [41,42,44,46]. In fig.1 we list the computed theoretical time dependence of polarization for GeO molecule in an electromagnetic field in a chaotic regime. In order to perform numerical analysis of the systems dynamics we used an advanced generalized techniques such as the wavelet analysis, multi-fractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, the Lyapunov exponent's (LE) analysis, and surrogate data method, prediction models etc [4-16]. The further step is an analysis of the corresponding time series (with the time step Dt=4×10^{-14}s). In Table 1 we list the computed values of the correlation dimension d_2, embedding dimension d_N , which are computed on the basis of the of false nearest neighbouring points algorithm with noting (%) of false points for different values of the lag time t. Accordingly in Table 2 we list the computed values of the Kaplan-York attractor dimension (d_L), LE (l_i, i=1-3) and the Kolmogorov entropy (K_{entr}).

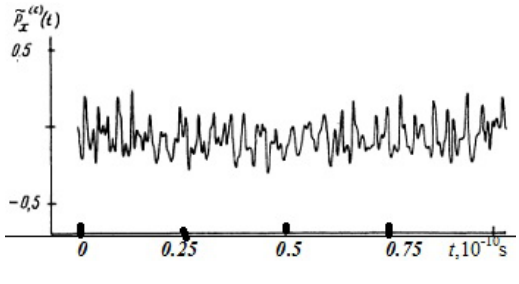

Figure 1. The computed characteristic time dependence of polarization of the GeO molecule in a field in a chaotic regime (see parameters in text).

Table 1.

The correlation dimension d_2, embedding dimension d_N, which are computed on the basis of the of false nearest neighbouring points algorithm with noting (%) of false points for different values of the lag time t

τ	d_2	(d_N)
42	3.04	5 (4.2)
4	2.73	3 (1.1)
6	2.73	3 (1.1)

Table 2.

The Kaplan-York attractor dimension (d_L), LE (l_i, i=1-3) and the Kolmogorov entropy (K_{entr})

λ_1	λ_2	λ_3	d_L	K_{entr}
0.146	0.0179	-0.321	2.51	0.16

Analysis of the received data on the LE, correlation, Kaplan York dimensions, Kolmogorov entropy etc shows that the dynamics of the Geo molecules in an electric field has the elements of a deterministic chaos (low-D strange attractor) and this conclusion is entirely agreed with the results of the classical-dynamical treating [18]. It is important to note that the Kaplan-York dimension is less than the embedding one confirming the correctness of the choice of the latter.

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This article has been received in May 2016.

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Abstract

It has been numerically studied a chaotic dynamics of diatomic molecules (on example of the GeO molecule in an infrared field) and some laser systems. An advanced generalized techniques such as the wavelet analysis, multi-fractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, the Lyapunov exponent's (LE) analysis, and surrogate data method, prediction models etc is used. It has been shown that systems exhibit a nonlinear behaviour with elements of a low-or high-dimensional chaos. There are firstly presented the numerical data on topological and dynamical invariants of chaotic systems, in particular, the correlation, embedding, Kaplan-York dimensions, LE, Kolmogorov's entropy etc for GeO molecule in an electromagnetic infrared field in the chaotic regime.

Key words: molecular system, electromagnetic field, chaotic dynamics

УДК 539.184, 539.186

А. В. Игнатенко, А. А. Кузнецова, А. С. Квасикова, А. В. Глушков, М. Ю. Гурская

НЕЛИНЕЙНАЯ ХАОТИЧЕСКАЯ ДИНАМИКА АТОМНЫХ И МОЛЕКУЛЯРНЫХ СИСТЕМ В ЭЛЕКТРОМАГНИТНОМ ПОЛЕ

Резюме

Представлены результаты численного анализа и моделирования хаотической динамики двухатомных молекул (на примере молекулы GeO) во внешнем электромагнитном (инфракрасном) поле. В анализе использованы эффективные версии таких методов анализа как мультифрактальный и вейвлет-анализ, метод корреляционного интеграла, алгоритмы средней взаимной информации, ложных ближайших соседей, суррогатных данных анализ показателей Ляпунова, энтропии Колмогорова,

спектральные методы и т.д. Показано, что двухатомная система в электромагнитном поле демонстрируют нелинейное поведение с элементами динамического хаоса. Представлены численные данные о топологических и динамических инвариантов системы в хаотическом режиме, в частности, корреляционной размерности, размерностей вложения, Каплана-Йорка, показателей Ляпунова, энтропии Колмогорова энтропия и т.д. для молекулы GeO в электромагнитном инфракрасном поле в хаотическом режиме.

Ключевые слова: молекулярная система, электромагнитное поле, хаотическая динамика,

УДК 539.184, 539.186

Г. В. Ігнатенко, А. О. Кузнецова, А. С. Квасикова, О. В. Глушков, М. Ю. Гурська

НЕЛІНІЙНИХ ХАОТИЧНА ДИНАМІКА АТОМНИХ ТА МОЛЕКУЛЯРНИХ СИСТЕМ В ЕЛЕКТРОМАГНІТНОМУ ПОЛІ

Резюме

Представлені результати чисельного аналізу і моделювання хаотичної динаміки двоатомних молекул (на прикладі молекули GeO) в зовнішньому електромагнітному (інфрачервоному) поле. В аналізі використані ефективні версії таких методів аналізу як мультіфрактальний і вейвлет-аналіз, метод кореляційного інтеграла, алгоритми середньої взаємної інформації, помилкових найближчих сусідів, сурогатних даних аналіз показників Ляпунова, ентропії Колмогорова, спектральні методи і т.і. Показано, що двоатомна система в електромагнітному полі демонструє нелінійне поведінку з елементами динамічного хаосу. Представлені чисельні дані по топологічним і динамічним інваріантам системи в хаотичному режимі, зокрема, кореляційної розмірності, розмірності вкладення, Каплана-Йорка, показників Ляпунова, ентропії Колмогорова тощо для молекули GeO в електромагнітному інфрачервоному поле в хаотичному режимі.

Ключові слова: молекулярна система, електромагнітне поле, хаотична динаміка