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CHAOTIC DYNAMICS OF DIATOMIC MOLECULES IN AN ELECTROMAGNETIC FIELD

Nonlinear chaotic dynamics of the diatomic molecules interacting with a resonant linearly polarized electromagnetic field is computationally modelled. It is presented an effective quantum-mechanical model for diatomic molecule in an electromagnetic field, based on the Schrödinger equation and model potential method. To detect the elements of a chaotic dynamics, we used the known chaos theory and non-linear analysis methods such as a correlation integral algorithm, the Lyapunov's exponents and Kolmogorov entropy analysis, prediction model etc. There are listed the data of computing dynamical and topological invariants such as the correlation, embedding and Kaplan-Yorke dimensions, Lyapunov's exponents, Kolmogorov entropy etc, for polarization time series of the ZrO molecule interacting with a linearly polarized electromagnetic field. The results obtained are in a physically reasonable agreement with the conclusions by Berman, Kolovskii, Zaslavsky, Zganh et al, Glushkov et al.

Introduction

Theoretical and experimental studying regular and chaotic dynamics of nonlinear processes in the different classes of quantum systems (in particular, atomic and molecular systems in an external electromagnetic field) attracts a great interest that is of a significant importance for multiple scientific and technical applications etc [1-70]. Some of the beauty of quantum chaos is that it has developed a set of tools which have found applications in a large variety of different physical contexts, ranging from atomic, molecular and nuclear physics (Chirijov, 1979, Delande-Gay 1986, Wintgen-Friedrich 1986, Wintgen 1987, Zaslavsky, Berman, Kolovsky, 1988, 1992, Meredith et al, 1988, Chelkowski et al, 1991, Delande et al 1991, Zhang, Katsouleas, Joshi, 1993, Cassati et al 1994, Glushkov et al 1993, 1997, 2014, Bohigas and Leboeuf 2002, Olofsson et al 2006, López, Mercado, 2015 et al), optical (Nockel-Stone 1997, Gmachl et al 1998) or microwave (Stockmann and Stein 1990, Sridhar 1991, Alt et al 1995, Kudrolli et al 1995, Pradhan and Sridhar 2000) resonators and mesoscopic physics (Richter et al 1996b, Richter 2000, Alhassid 2000, Glushkov et al, 2005-2007) and others (see review [11]). New field of investigations of the quantum and other systems has been provided by the known progress in a development of a nonlinear analysis and chaos theory methods [1-12,17-30]. In Refs. [11,27-33] the authors applied different approaches to quantitative studying regular and chaotic dynamics of atomic and molecular systems interacting with a strong electromagnetic field and laser systems. The most popular approach includes the combined using the advanced nonlinear analysis and a chaos theory methods such as the autocorrelation function method, multifractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov exponent's analysis, surrogate data method, stochastic propagators method, memory and Green's functions approaches etc (see details in Refs. [17-33]).

In this paper we present the results of computing chaotic dynamics of the concrete molecular systems (diatomic molecules) interacting with a linearly polarized resonant electromagnetic field. The quantum-dynamic approach to diatomic molecule in an electromagnetic field

is used and based on the solution of the time-dependent Schrödinger equation, optimized operator perturbation theory and realistic model potential method.

2. Quantum-dynamical and chaos-geometric modeling dynamics of diatomic molecule in a field

Below we briefly consider a quantum dynamical approach to studying a regular and chaotic dynamics of diatomic molecules in a resonant electromagnetic field [11]. It is based on the numerical solution of the time-dependent Schrödinger equation and realistic Simons-Parr-Finlan model for the diatomic molecule potential $U(x)$. The Simons-Parr-Finlan formulae for the molecular potential is:

$$( ) \quad _0[\quad)/ \ ]^2\{1 \ \sum \ [\tag{1a}$$

or introducing $x = r - r_0$:

$$( ) \quad _0[\ (\quad _0]^2\{1 \ \sum \ [\ (\quad _0 \tag{1b}$$

where the coefficients b_i are linked with corresponding molecular constants.

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

$$i\partial\Psi / \partial t = [H_0 + U(x) - d(x)E_M\varepsilon(t)\cos(\omega_L t)]\Psi \tag{2}$$

where E_M - the maximum field strength, $\varepsilon(t)=E_0 cos(\nu t)$ 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:

$$P_x(t) = p_c^{(x)}(t)cos\omega t + p_s^{(x)}(t)sin\omega t, \tag{3a}$$

$$P_y(t) = p_c^{(y)}(t)cos\omega t + p_s^{(y)}(t)sin\omega t, \tag{3b}$$

$$p_c^{(x,y)}(t) = \left(\frac{1}{T}\right)\oint\langle\psi(t)|\hat{d}_{x,y}|\psi(t)\rangle cos\omega t dt, \tag{3c}$$

where T — period of the external field, d –dipole moment. As usually, the power spectrum can be further determined as follows:

$$S(\omega) = |F[p(t)]|^2. \tag{4}$$

To avoid the numerical noise during the Fourier transformation, the attenuation technique used,i.e. at $t > t_p$, $p(t)$ is replaced by

$$p(t)cos^2\{\pi(t - t_p)/[2(T - t_p)]\}, \quad (t_p < t < T) \tag{5}$$

with $T=1.5t_p$.

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 [7-12].

The theoretical foundations of the universal approach to analysis of chaotic dynamics of the quantum systems in an electromagnetic field have been presented earlier (see, c.g., [11,17-33]). Here we are limited only by the key moments. Generally speaking, the approach includes a set of such non-linear analysis and a chaos theory methods as the correlation integral approach, multi-fractal and wavelet analysis, average mutual information, surrogate data, Lyapunov's exponents and Kolmogorov entropy approach, spectral methods, nonlinear prediction (predicted trajectories, neural network etc) algorithms.

The goal of the embedding dimension determination is to reconstruct a Euclidean space R^d large enough so that the set of points d_A can be unfolded without ambiguity. 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. $d_E > d_A$. There are several standard approaches to reconstruction of the attractor dimension (see, e.g., [17-33]). The correlation integral analysis is one of the widely used techniques to investigate the signatures of

chaos in a time series. The analysis uses the correlation integral, $C(r)$, to distinguish between chaotic and stochastic systems.

To compute the correlation integral, the algorithm of Grassberger and Procaccia [24] is the most commonly used approach. According to this algorithm, the correlation integral is

$$C(r) = \lim_{N\to\infty} \frac{2}{N(n-1)} \sum_{\substack{i,j \\ (1\le i<j\le N)}} H\left(r - |\,\mathbf{y}_i - \mathbf{y}_j\,|\right) \qquad (6)$$

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. To verify the results obtained by the correlation integral analysis, one could use the surrogate data method. This approach makes use of the substitute data generated in accordance to the probabilistic structure underlying the original data.

The important dynamical invariants of a chaotic system are the Lyapunov's exponents (see, c.g., [11,25-30]). They are usually defined as asymptotic average rates, they are independent of the initial conditions, and therefore they do comprise an invariant measure of attractor. Saying simply, the Lyapunov's exponents are a parameter to detect whether the system is chaotic or not.

The Kolmogorov entropy K_{ent} measures the average rate at which information about the state is lost with time. An estimate of this measure is the sum of the positive Lyapunov's exponents. The estimate of the dimension of the attractor is provided by the Kaplan and York conjecture:

$$d_L = j + \frac{\sum_{\alpha=1}^{j} \lambda_\alpha}{|\,\lambda_{j+1}\,|}, \qquad (7)$$

where j is such that $\sum$ and $\sum$, and the Lyapunov's exponents λ_α are taken in descending order.

There are a few approaches to computing the Lyapunov's exponents. One of them computes the whole spectrum and is based on the Jacobi matrix of system. In our work we use the method with the linear fitted map proposed by Sano and Sawada [58], although the maps with higher order polynomials can be also used.

3. Some results and conclusions

Here we present the results of numerical simulation of the time dynamics for diatomic molecule ZrO in the electromagnetic field. An electromagnetic field is characterized by the parameter: $S = cE/8\pi$. where c is the velocity of light and E is a field strength. The parameter W of interaction of an electromagnetic radiation with a molecule is as follows:

$$W[cm^{-1}] = 120.3(d_0 / r_0)(S / M\omega_e)^{1/2} \qquad (8)$$

where 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 . In Table 1 we list a set of the ZrO molecules and field parameters [68-70].

The corresponding Chirikov parameter [10] in this case is as: $\delta n = 2(Ed/B)^{\frac{1}{2}} \gg 1$. The typical theoretical time dependence of polarization for ZrO molecule in the field in a chaotic regime is presented in Ref. [11]. The concrete step is an analysis of the corresponding time series with the n=7.6×10^3 and Δt=5×10^{-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 1.

Set of the ZrO molecular constants and electromagnetic field parameters

Parameters	ZrO
ω_e= (cm^{-1})	969.7
$\omega_e x_e$= (cm^{-1})	4.90
B_e (cm^{-1})	0.423
D_e (cm^{-1})	3.19×10^{-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.

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}

d_2	λ_1	λ_2	d_L	K_{entr}	K_{GW}
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 [3,7-11].

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CHAOTIC DYNAMICS OF DIATOMIC MOLECULES IN AN ELECTROMAGNETIC FIELD

Summary

Nonlinear chaotic dynamics of the diatomic molecules interacting with a resonant linearly polarized electromagnetic field is computationally modelled. It is presented an effective quantum-mechanical model for diatomic molecule in an electromagnetic field, based on the Schrödinger equation and model potential method. To detect the elements of a chaotic dynamics, we used the known chaos theory and non-linear analysis methods such as a correlation integral algorithm, the Lyapunov's exponents and Kolmogorov entropy analysis, prediction model etc. There are listed the data of computing dynamical and topological invariants such as the correlation, embedding and Kaplan-Yorke dimensions, Lyapunov's exponents, Kolmogorov entropy etc, for polarization time series of the ZrO molecule interacting with a linearly polarized electromagnetic field. The results obtained are in a physically reasonable agreement with the conclusions by Berman, Kolovskii, Zaslavsky, Zganh et al, Glushkov et al.

Key words: Nonlinear chaotic dynamics, diatomic molecules, electromagnetic field

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ХАОТИЧЕСКАЯ ДИНАМИКА ДВУХАТОМНЫХ МОЛЕКУЛ В ЭЛЕКТРОМАГНИТНОМ ПОЛЕ

Резюме

Моделируется нелинейная хаотическая динамика двухатомных молекул, взаимодействующих с резонансным линейно-поляризованным электромагнитным полем. Представлена эффективная квантово-механическая модель для двухатомной молекулы в электромагнитном поле, базирующаяся на использовании уравнения Шредингера и метода модельного потенциала. Для детектирования элементов хаотической динамики использованы методы теории хаоса и нелинейного анализа, такие как алгоритм корреляционного интеграла, анализ на основе показателей Ляпунова и энтропии Колмогорова, траекторная модель прогноза и др. Представлены данные вычисления динамических и топологических инвариантов таких как корреляционная размерность, размерности вложения и Каплана-Йорка, показатели Ляпунова, энтропия Колмогорова и т. д. для временной зависимости поляризации молекулы ZrO, взаимодействующей с линейно-поляризованным электромагнитным полем. Полученные результаты находятся в физически разумном согласии с качественными выводами Бермана, Коловского, Заславского, Згана, Глушкова и др.

Ключевые слова: нелинейная хаотическая динамика, двухатомная молекула, электромагнитное поле

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ХАОТИЧНА ДИНАМІКА ДВОАТОМНИХ МОЛЕКУЛ В ЕЛЕКТРОМАГНІТНОМУ ПОЛІ

Резюме

Моделюється нелінійна хаотична динаміка двоатомних молекул, взаємодіючих з резонансним лінійно-поляризованим електромагнітним полем. Представлена ефективна квантово-механічна модель для двоатомних молекули в електромагнітному полі, що базується на використанні рівняння Шредінгера і методу модельного потенціалу. Для детектування елементів хаотичної динаміки використані методи теорії хаосу і нелінійного аналізу, такі як алгоритм кореляційного інтеграла, аналіз на основі показників Ляпунова і ентропії Колмогорова, траєкторна модель прогнозу і ін. Представлені дані обчислення динамічних і топологічних інваріантів таких як кореляційна розмірність, розмірності вкладення і Каплана -Йорка, показники Ляпунова, ентропія Колмогорова і т. д. для часової залежності поляризації молекули ZrO, яка взаємодіє з лінійно-полярізованим електромагнітним полем. Отримані результати знаходяться в фізично розумній згоді з якісними висновками Бермана, Коловського, Заславського, Згана, Глушкова та ін.

Ключові слова: нелінійна хаотична динаміка, двоатомна молекула, електромагнітне поле