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STOCHASTIC DYNAMICS OF THE LASER FIELD ROTATIONAL EXCITATION FOR MOLECULES

A advanced multi-level optimized stochastic model for definition of the optimal form of laser pulse to reach the maximal effectiveness of laser action in process of selective molecule excitation and ionization is used in calculation the parameters of the optimal excitation for molecule. It is estimated dependence (number of particles) of functional of the quality on the rotational energy and wave length of laser radiation

At present time it is of a great important development of an effective advanced multi-level optimized stochastic models for definition of the optimal form of laser pulse to reach the maximal effectiveness of laser action in process of selective molecule excitation and ionization. The purpose is to calculate the parameters of the optimal excitation for molecule [1-10]. This topic represents a significant theoretical and applied interest for many physical, chemical branches such as an atomic, molecular physics, quantum electronics, physics of elements, devices, sensor technologies, plasmochenistry laser photochemistry and biology. One could remind about physical basis for creation and construction of special devices for sensing physical, chemical properties of the molecular systems and at last their application in the nano-electronics, nano-atomic optics, quantum computing, molecular sensors technologies etc.

As it was indicated in Refs. [1-10], a great perspectives has the studied topic for many problems of laser photochemistry. Letokhov et al [2,3] experimentally studied possibility of cleaning the substance in a gas phase by means of the photoionization or photo dissociation of admix- tured molecules in IR laser field on the example of cleaning $AsCl_3$ from admixtures C_1H_4Cl2 and CCl_4.From theoretical and experimental points of view, it is very important theoretical and experimental studying optimal realizations of processes of the multi-step and multi photon excitation and ionization, dissociation. Though many of cited processes are quite satisfactorily described (at least, at qualitative level) by simplified models. A majority of tasks for action of laser radiation and high intensive particles beams on molecular gases are quite acceptably described by multilevel stochastic models, which result in systems of differential equations or differential equation in partial derivatives of the Focker-Plank type [3,7,8,14]. Nowdays a consistent theory of the optimal realizations of these processes is absent. In refs. [12-15] a new multi-level optimized model for definition of the optimal form of laser pulse to reach the maximal effectiveness of laser action in process of selective excitation and ionization of molecules has been proposed. Further within the optimal governing theory a problem of optimization for electron, vibtational and rotational excitation, photo ionization and dissociation in a laser field was studied and As example, the parameters of the optimal excitation and ionization for molecules HCl, $CF_3Br(I)$, SiH_4 etc. have been determined. Here we consider a generalized advanced stochastic model for definition of the optimal form

of laser pulse to reach the: maximal effectiveness of laser action in process of selective molecule excitation and ionization, which generalizes earlier formulated approaches [13-15].

As usually, we start from the stochastic differential equation of the Focker-Plank type:

$$\partial f / \partial t = L_{RT} + L_u(f, I) \qquad (1)$$

where f is a density of molecules at a chosen vibrated level with rotational energy x; I is a laser pulse intensity; L_{RT},$L_\mu(f,I)$ are operators, which describe the RT relaxation and laser radiation action and have the standard form:

$$L_{RT}(f) = \partial^2 f/\partial x^2 + \partial f/\partial x, \ldots, L_u = I(x,t)u(t)(f(x_2,t) - f(x_1,t)) \qquad (2)$$

At initial moment of time there is some initial distribution $f(x,0)$, and for t>0 syste m is ex cited by resonance laser fieldwith frequency, which is resonant to rotati on al transition $x_1 \to x_2$

Frequency of the exciting field is considered as as governing parameter. To estimate an effectiveness of action one must study a quality functional, which characterises a distribution of molecules on rotational energies to moment t_1

$$Y(u) = \int_0^R f(x, t_1; u)h(x)dx \qquad (3)$$

where $h(x)$ is some function, which corresponds to required form of the final distribution.

Further we are dealing with real form of the laser pulse. In refs. [12-15] we deal with a multi-level optimized model for definition of the optimal form of laser pulse. In fact it has been used the pulse in a Lorenze form. Here we consider firstly the pulse in the Gaussian form. Further we used the standard procedure of the governing theory The optimal governing task for definition of the optimal laser pulse form to achieve a maximal laser action effectiveness is written as follows [15]:

$$\partial f / \partial t = \partial^2 f/\partial x^2 + \partial f/\partial x + I(x,t)u(t)(f(x_2,t) - f(x_1,t))$$
$$f(x,0) = f_0(x), \ldots\ldots\ldots 0 < x < R, \qquad (4)$$
$$\partial f/\partial x + + f|_{x=0,R} = 0, \ldots 0 < t < t_1$$

Following to Ref.[14,15], we use the necessary condition of optimality, i.e. if $(x_1^*,\ x_2^*)$ is an optimal goveming for functional (3) and $f^*(x,t)$ $\psi^*(x,t)$ are corresponding solutions, then we have the following condition for any x_1, x_2 from interval [0, R]:

$$Y'_{x_1}(x_1^*, x_2^*, f^*, \Psi^*)(x_1 - x_1^*) + Y'_{x_2}(x_1^*, x_2^*, f^*, \Psi^*)(x_2 - x_2^*) \le 0$$

D ependence (number of partiel es) in the interval of energies xI[x_1, x_2] (in units of kT) upon x_1 and wave length of laser radiation, which is corresponding to rotation transition x_1 ® x_2, is determined by the functional:

$$I(u) = \int_0^R f(x, t_1; x_1, x_2)h(x)dx \qquad (5)$$

Using the numerical methodics [14,15] we have carried out testing of the advanced model for molecules *HBr* (T=300 K, R=25; the values of parameters are taken from refs.[2-4, 16]). In figure 1 it is presented a dependence (number of particles) of the functional (5) in the interval of energies xI[13,25] (in un its of kT) upon x; and wave length of laser radiation, which is corresponding to rotation transition $x_1 \to x_2$. In exp re ssion (4) h is a function, which corresponds to required form of the final distribution $f(x,t,u)$, i.e. density ofmolecules at chosen vibration level, which has a rotational energy x at moment of time t; xe[ü, R). The obtai ned data are qualitatively similar to resultsof ref. [14 ,1 5] for molecule *HCl*, CF_3Br. The quantitative difference (-5%) is providedby using the real laser pulse form (3) and corrected molecular constants set. Probably, this difference should be in mo re details analyzed with accounting for the possible photon-correlation stochastic effects.

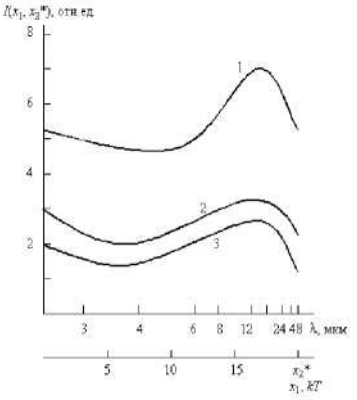

Fig. 1. Dependence of the functional $I(x_1, x_2)$ upon x_1 and wave length of laser radiation for $t_1=2t_R$ (1), $t_1=4t_R$ (2), $t_1=6t_R$ (3) for molecule HBr (see text).

References

1. Lambert J.D.,Vibrational and Rotational Relaxation in Gases (Oxford.-1997).
2. Letokhov V.S., Nonlinear selective photo-processes in atoms and molecules (Moscow.- 2003).
3. Bagratashvili V.N., Letokhov V.S., Makarov A.A., Ryabov E.A., Multiphoton processes in molecules in IR la-serfield(Moscow.- 1991).
4. Goldansky V.I., Letokhov VS. Effect of laser radiation on nuclear decay processes// Sov. Phys. JETP.-1994.- Vol.67.-P.513-516.
5. Ivanov L.N., Letokhov VS. Spectroscopy of autoionization resonances in heavy elements atoms// Com. Mod. Phys.D.:At. Mol.Phys.-1995.- Vol.4.-P. 169-184.
6. Glushkov A.V., Ivanov L.N. Radiation Decay of Atomic States: atomic residue and gauge non-invariant contributions // Phys. Lett.A.-1992.- Vol.170,N1.-P.33-37.
7. Panchenko V.Ya., Tolstoshein A.Yu., Optimization of condition of the ritation- al excitation for molecular gas// Soviet Chem.Phys.-1997.-Vol.6.-P.16-20.
8. Laptev V.B., Ryabov E.A., Isotopically-selective dissociation BCl_3 in a two-colour IR laser field// Soviet Chem. Phys.- 1998.-Vol.7,N2.-P. 165-170.
9. Glushkov A.V., Malinovskaya S.V., Co-operative laser nuclear processes: border lines effects// In: New projects of research in nuclear physics. Eds. G.Fazio, F.Hanappe, (Singapore, World Sci.- 2003).-P.242-250.
10. Glushkov A.V., Ambrosov S.V., Ignatenko A.V., Korchevsky D.A., DC Strong Field Stark Effect for Non- hydrogenic Atoms//Int.Journ.Quant. Chem.-2004.-Vol.99,N5.-P.936-939.
11. Glushkov A.V., Malinovskaya S.V., Shpinareva I. etal, Diagnostics of col-lisionally pumped plasma & search of optimal plasma parameters for x-ray lasing//J.Phys.CS.-2005.-Vol.11-P.188-198.
12. Glushkov A.V., Prepelitsa G.P., Svinarenko A.A. Sensing the stochastic laser pulse structure and chaotic and photon-correlation effects in the nonlinear multi-photon atomic dynamics in laser and DC electric field// Sensor Electr. & Microsyst. Techn.-2004.-N2.-P.89-95
13. Glushkov A.V., Malinovskaya S.V., Shpinareva I.M., Kozlovskaya V.P., Gura V.I. Quantum stochastic modelling multi-photon excitation and dissociation for CF_3Br molecules: An effect of rotational and V-T relaxation // Int. Journ. Quant. Chem.-2005.-Vol. 104,N4.- P.562-570.
14. Loboda A. , Glushkov A.V., Shpinareva I. et al, Optimization of laser field rotational excitation of molecules and its possible use in the selective photoionization method for cleansing semiconductor surface// Surface and Interface Analysis.-2005.-Vol.16.-P.931-935.
15. Shpinareva I.M., Sensing a dynamics of the laser field rotational excitation for molecules and possible using in laser photoionization cleaning semiconductor surfaces//Sensor Electr and Microsystems Techn.-2005.- N4.-P.22-26.
16. Glushkov A.V., Ambrosov S.V., Shpinareva I.M., etal, Spectroscopy of diatomic van-der-waals molecules: atom of inert gas- atom of galogen// Opt.Spectr.-1998.-Vol.84.-P.567-572.

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Abstract. An advanced multi-level optimized stochastic model for definition of the optimal form of laser pulse to reach the maximal effectiveness of laser action in process of selective molecule excitation and ionization is used in calculation the parameters of the optimal excitation for molecule. It is calculated dependence (number of particles) of functional of the quality on the rotational energy and wave length of laser radiation.

Key words: rotational excitation, molecules in a laser field, stochastic modelling

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СТОХАСТИЧЕСКАЯ ДИНАМИКА ВРАЩАТЕЛЬНОГО ВОЗБУЖДЕНИЯ МОЛЕКУЛ В ПОЛЕ ЛАЗЕРНОГО ИЗЛУЧЕНИЯ

Резюме. Обобщенная многоуровневая оптимизационная стохастическая модель определения оптимальной формы лазерного импульса для достижения максимальной эффективности лазерного воздействия в процессе селективного возбуждения и ионизации молекул использована в оценке параметров оптимального вращательного возбуждения молекул. Рассчитана зависимость функционала качества (число частиц) от величины вращательной энергии и длины волны лазерного излучения.

Ключевые слова: вращательного возбуждения, молекулы в поле лазерного излучения, стохастическая модель

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СТОХАСТИЧНА ДИНАМІКА РОТАЦІЙНОГО ЗБУДЖЕННЯ МОЛЕКУЛ У ПОЛІ ЛАЗЕРНОГО ВИПРОМІНЮВАННЯ:

Резюме. Узагальнена багаторівнева оптимізаційна стохастична модель визначення оптимальної форми лазерного імпульсу для досягнення максимальної ефективності лазерної дії у процесі селективного збудження та іонізації молекул використана у розрахунку параметрів оптимального збудження молекул. Оцінена залежність функціоналу якості (число частинок) від величини ротаційної енергії та довжини хвилі лазерного випромінювання.

Ключові слова: ротаційне збудження, молекули у лазерному полі, стохастична модель