CONTROL OF QUANTUM AND CLASSICAL MOLECULAR DYNAMICS

M.S. Ananyevskiy, A.A. Efimov, * **A.A. Fradkov** **

* *St.Petersburg State University,*
28 Universitetskii Prospekt, 188194, Russia
e-mail: soomrack@pisem.net
** *Institute for Problems of Mechanical Engineering.*

Abstract: Two examples of application of nonlinear control methods to control of molecular motion are studied. Firstly, the problem of controlling quantum observables for a finite dimensional model of a diatomic molecule is examined and a new control law is obtained based on speed-gradient approach. A substantial domain of initial conditions in the phase space ensuring achievement of the control goal is determined. The results are illustrated by the numerical example for Hydrogen fluoride molecule. Secondly, an approach to dissociation control of a 3-atomic molecules with straight valence angle is proposed based on speed-gradient method. A connection between dissociation and synchronization of bond dynamics are analyzed by computer simulations for 3-atomic HCN molecule. The presented problems and their solutions demonstrate a broad range and prospects of potential applications of nonlinear control methods to control of molecular systems. *Copyright © 2005 IFAC.*

Keywords: Energy control, Speed gradient, Quantum mechanics, Nonlinear control, molecular dynamics

1. INTRODUCTION

Since the beginning of the 1990s a growing interest has been observed in control problems for molecular systems. According to Science Citation Index, the number of papers devoted to quantum control in 1991-2002 reached 3800, and the number of articles published in 2003 exceeds 600. Practical realization of different control principles has become possible recently thanks to development of fast femtoseconds pulse lasers. Using advanced control methods for changing natural course of chemical reactions, controlling them and developing new chemical technologies is studied by many authors, see (Brown and Rabitz, 2002; Butkovsky and Samoilenko, 1980).

In this paper two examples of application of nonlinear control methods to control of molecular motion are studied.

In the first part (Sections 2,3,4) the control of observables problem is examined based on finite dimensional quantum-mechanical description of molecular dynamics. Compared to papers (Ananjevsky et al, 2003; Krempl et al, 1992), where control function is constructed using classical description in this paper the control algorithm is constructed by applying Speed-Gradient method for quantum model. It is proved that the control goal is attained for initial condition in a sufficiently large domain of phase space. The control function can be arbitrarily small. The effi-

---

[1] Supported by Russian Foundation of Basic Research (grant RFBR 05-01-00869), Complex Program of the Presidium of RAS No 19 “Control of mechanical systems” and Program “Development of research potential of Higher School” of the Ministry of Education and Science of RF.

ciency of control algorithm is illustrated by the numerical example for Hydrogen fluoride (HF) molecule.

In the second part (Sections 5,6) a nonlinear oscillator model with Morse potential is considered as the mathematical model of molecular dynamics. An approach to dissociation control of a 3-atomic molecules with straight valence angle is proposed based on speed-gradient method. A connection between dissociation and synchronization of bond dynamics are analyzed by computer simulations for 3-atomic HCN molecule.

2. QUANTUM MODEL OF A DIATOMIC MOLECULE

The following mathematical model of a controlled quantum system is considered. It describes diatomic molecule with Morse potential (Krempl et al, 1992) (Hartree units):

$$i\frac{\partial\Phi(t,r)}{\partial t} = -\frac{1}{2M}\frac{\partial^2\Phi(t,r)}{\partial r^2} + V(r)\Phi(t,r) + uAr\Phi(t,r), \tag{1}$$

$$V(r) = D(\exp(2\alpha\frac{r_0-r}{r_0}) - 2\exp(\alpha\frac{r_0-r}{r_0})), \tag{2}$$

where $i = \sqrt{-1}$ — imaginary unit; $\Phi(t,r)$ — wave function, for any time instant t_0: $\Phi(t_0,r) \in L^2(0,+\infty)$; r — distance between atoms of molecule, $r \in (0,+\infty)$; $V(r)$ — Morse potential; M,A,D,α,r_0 — constants, which depend on specific molecule.

A finite level approximation by eigenfunctions $\phi_k(r)$ of unperturbed Schrodinger operator: $H_0 = -\frac{1}{2M}\frac{\partial^2}{\partial r^2} + V(r)$, corresponding to undissociated molecule states is used. Eigenfunctions and eigenvalues are analytically given (Flugge, 1971). All eigenvalues corresponding to undissociated molecule states can be calculated with a high precision using the following expressions:

$$\lambda_k = -D + \frac{1}{2Mr_0^2}\left(\alpha\sqrt{8MDr_0^2}\left(k+\frac{1}{2}\right) - \alpha^2\left(k+\frac{1}{2}\right)^2\right), \quad 0 \le k < \frac{\sqrt{2MDr_0^2}}{\alpha} - \frac{1}{2}, \tag{3}$$

eigenfunctions $\phi_k(r)$ corresponding to eigenvalues λ_k:

$$\phi_k(r) = B_k y^{-\frac{m_k}{2}} e^{\frac{1}{2}y} \frac{d^k}{dy^k}\left(y^{m_k+k}e^{-y}\right),$$

$$y = \sqrt{\frac{8MDr_0^2}{\alpha^2}} e^{-\alpha\frac{r-r_0}{r_0}}, m_k = \frac{\sqrt{-8M\lambda_k r_0^2}}{\alpha}. \tag{4}$$

Normalized factors B_k are calculated numerically using MATLAB. The finite level approximation yields the following mathematical model of diatomic molecule:

$$i\dot{\phi}(t) = H_0\phi(t) + u(t)H_1\phi(t), \quad \phi(t) \in \mathbb{C}^n, \tag{5}$$

where $\phi(t)$ — coefficient vector of wave function decomposition $\Phi(t,r)$ in n eigenfunctions; H_0 — diagonal matrix, element (k,k) is λ_k; H_1 — matrix corresponding to operator of control. The element (k,m) of H_1 can be calculated using the following expression: $A\int_0^{+\infty} r\phi_k(r)\phi_m(r)dr$.

The problem is to design the control function $u(t)$ to obtain the convergence to the goal value Z_g of observable $Z(t) = \phi(t)^*Z\phi(t)$ of quantum system (5):

$$\lim_{t\to+\infty} \phi(t)^*Z\phi(t) = Z_g. \tag{6}$$

3. CONTROL ALGORITHM DESIGN

It is suggested to use Speed-Gradient algorithm in finite form (Fradkov et al, 1999) for designing the control function. The following goal function is introduced (it doesn't change while $u = 0$):

$$Q(\phi) = \left(\phi^*Z\phi - Z_g\right)^2, \qquad \phi \in \mathbb{C}^n. \tag{7}$$

The convergence to zero of the goal function is equivalent to achievement of the control goal. According to speed-gradient method the control algorithm is chosen to ensure nonpositivity of the derivative of the goal function along trajectories of controlled system (5) : $u = -\nabla_u\dot{Q}(\phi)$, here dot means derivative along trajectories of the system (5), and ∇_u - gradient by parameter u.

$$u = -\nabla_u\dot{Q}(\phi) = -\nabla_u[2(\phi^*Z\phi - Z_g)(i(H_0\phi + uH_1\phi)^*Z\phi - i\phi^*Z(H_0\phi + uH_1\phi))] \tag{8}$$

Assume that the observable Z commute with operator H_0. The following algorithm for controlling observables of diatomic molecule is proposed:

$$i\dot{\phi}(t) = H_0\phi(t) + uH_1\phi(t), \tag{9}$$

$$u = 2(\phi(t)^*Z\phi(t) - Z_g)(\phi(t)^*\{Z,H_1\}_\hbar\phi(t)), \tag{10}$$

where $\{\cdot,\cdot\}_\hbar$ — quantum Poisson bracket
($\{H_0,H_1\}_\hbar = \frac{i}{\hbar}[Z,H_1] = \frac{i}{\hbar}(ZH_1 - H_1Z)$).

The feedback algorithm for controlling observables was designed by applying Speed Gradient method to the quantum system (9). But in quantum systems feedback control is unrealizable because each measurement changes the state of the system (Brown and Rabitz, 2002). To use this algorithm the computer simulation is performed for calculating control as the time-depended function for known initial data. In the simulation section an example of such control function for energy of HF molecule is presented.

4. CONTROL ALGORITHM ANALYSIS

Impose the following restrictions on operators Z, H_0 and H_1:

A1) $z_k - z_m \neq 0$, $k \neq m$, $k,m = \overline{1,n}$ where z_k are eigenvalues of Z in ascending order;

A2) $(\lambda_k - \lambda_m) \neq (\lambda_r - \lambda_s)$, $(k,m) \neq (r,s)$, $k,m,r,s = \overline{1,n}$,

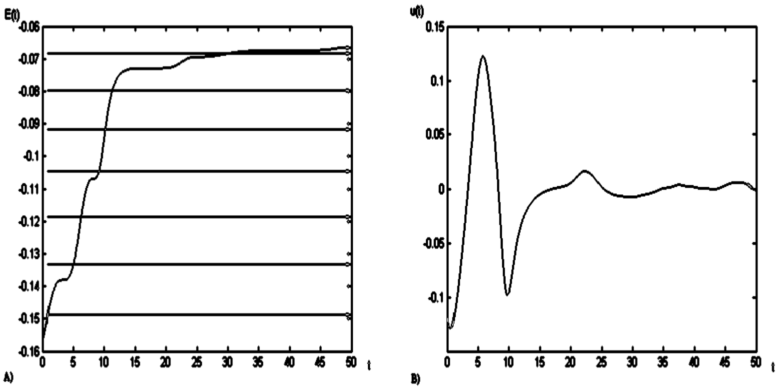

Fig. 1. a) Energy evolution (horizontal lines are energy levels); b) control function $u(t)$.

A3) $h_k H_1 h_m \neq 0$, $k, m = \overline{1,n}$, where h_k, $k = \overline{1,n}$ be linearly independent eigenvectors H_0.

The following theorem gives the mathematical basis for using algorithm (9) , (10).

Theorem 1. Consider the system (5) with feedback control law (10), where Z and H_0 commute. Given the assumptions A1), A2), A3) and $z_k < Z_g < z_{k+1}$. Then for any initial condition from $M = \{\phi : z_k < \phi^* Z \phi < z_{k+1}\}$ the goal (6) is achieved.

Proof. Since the evolution operator of system (9) , (10) is unitary, and the initial vector belongs to the unit sphere, the total trajectory also belongs to the unit sphere. Trajectory's continuability on $\mathbb{R}$ is the consequence of boundedness of the right part of equation (9). To proof the asymptotic stability the goal function $Q(\phi)$ is used as the Lyapunov function. Its derivative along the systems trajectories is nonpositive:

$$\dot{Q}(\phi) = -2(\phi^* Z \phi - Z_g)(\phi^* \{Z, H_1\}_\hbar \phi)$$

$$\times 2(\phi^* Z \phi - Z_g)(\phi^* \{Z, H_1\}_\hbar \phi), \qquad (11)$$

It follows from LaSalle's theorem that any system trajectory converges to maximal invariant subset of the set $K = \{\phi : \dot{Q}(\phi) = 0\}$.

Examine the maximal invariant subset of K. There are only two cases when $\dot{Q}(\phi)$ is equal to zero:

- $\phi^* Z \phi - Z_g = 0$,
- $\phi^* \{Z, H_1\}_\hbar \phi = 0$.

Let K_1 be a subset of phase space, where the first equation is true, K_2 be a subset where the second one is true ($K = K_1 \cup K_2$). The set K_1 is the invariant of the system (9). For any phase vector $\phi_1 : \phi_1^* Z \phi_1 - Z_g = 0$ and for any time instant t_0 function $\phi(t) = e^{H_0(t-t_0)}\phi_1$ is the trajectory of the system (9) , (10) and this trajectory belongs to K_1. Therefore, maximal invariant of K is the union of K_1 and maximal invariant of K_2. For trajectories belonging to K_2 it follows that the control function is equal to zero along whole trajectory, and any trajectory can be given by the following expression:

$$\phi(t) = \sum_{k=1}^{n} c_k exp(-i\lambda_k t) h_k, \quad \sum_{k=1}^{n} |c_k|^2 = 1. \quad (12)$$

Substitutiion of this expression into the equation of K_2 yields:

$$\sum_{k,m=1}^{n} c_k^* c_m (z_k - z_m) e^{i(\lambda_k - \lambda_m)t} h_k^* H_1 h_m = 0. \quad (13)$$

Due to condition A2) functions $\exp\left(i(\lambda_k - \lambda_m)t\right)$ are linear independent. Therefore, this linear combination is identically zero only if all the coefficients are zero. It follows from conditions A1), A2), A3) that only one of coefficients c_k, $k = \overline{1,n}$ can be nonzero. Hence, maximal invariant of K_2 is the set of pure states of the system (I(B) defines maximal invariant of set B):

$$I(K_2) = \{\phi : \phi = e^{ic} h_k, \quad k = \overline{1,n}, c \in \mathbb{R}\} \quad (14)$$

As long as goal function is nonincreasing, and its minimal value on elements of set $I(K_2)$ is $min_{k=\overline{1,n}}(z_k - Z_g)^2$, and the initial value of goal function is smaller then this minimum (minimum is not zero), the goal function converges to zero and the observable Z converges to the goal value Z_g. □

Remark 1. Simulation demonstrated that the control law (10) asymptotically drives observable Z to the goal value from any initial state (except pure states).

Remark 2. The theorem can be applied not only for diatomic molecule. The result can be useful for some quantum systems like (5).

Simulation results. Algorithm (9) , (10) was applied to energy control of molecule HF, described by equation (1). Constants for HF molecule are as follows (Krempl et al, 1992): $M = 1732$, $A = 0.4541$, $D = 0.2101$, $\alpha = 2.1350$, $r_0 = 1.75$ (Hartree units). Observable of energy is H_0: $E(t) = \phi(t)^* H_0 \phi(t)$. Molecular energy levels are energy of pure states. The initial value of phase vector is uniformly distributed between 3rd and 4th energy levels. In atomic units the initial energy is -0.1571. The goal value for energy is -0.06, it lies between 10th and 11th energy levels. The control function has the following form $F(x) = Kx$. Gain factor K is 200. Time for simulating is

50 femtoseconds (1fs $=10^{-15}$s). Figures (1) display energy evolution ($E(t)$) and control function ($u(t)$). The figures confirm efficiency of algorithm (9) , (10) for control of diatomic molecule observables. Also figures confirm that the area of stability is greater then the one for which theorem was proved.

5. CONTROL OF ENERGY AND SELECTIVE DISSOCIATION OF A MODEL 3-ATOMIC MOLECULE

Problem of purposeful changing and stabilization of energy of internal degrees of freedom in molecular systems is an important problem of laser chemistry. Processes of the bond excitation and dissociation in weak infrared laser fields have many applications, such as control of chemical reactions, chemical structure identification and others (Rice and Zhao, 2000). In the second part of the paper we concentrate at the process of controlled selective dissociation of strong bond in a 2-DOF model of HCN molecule with classical mechanical representation of molecular dynamics, suggesting some new approaches to the foregoing problems.

Although molecular motion is properly described by the Schrodinger equation, successful modelling for many molecular purposes can be done with classical mechanics. Thus, since the dissociation stage is characterized by the high values of energy, the results for classical and quantum-mechanical simulations of controlled dissociation are often similar (see, e.g. (Ananjevsky et al, 2003)). Often control design for quantum-mechanical ensembles is very complicated. Therefore we study the controlled selective dissociation for the model of molecule, based on classical mechanical representation of the intramolecular dynamics.

The 3-atomic molecule HCN in external laser field is modelled as two kinetically and potentially coupled Morse oscillators with collinear orientation, interacting with the field. Effects of bending, rotation and changing orientation are neglected. These additional degrees of freedom, surely, can play a role, but in sufficiently intense external fields such molecule tends to align along the field corresponding to a quasi-linear model for the controlled motion (**?**).

Despite all these simplifications, there are some fundamental difficulties in a model analysis:

1. strong nonlinearity (so the oscillations frequency depend on the energy and superposition principle do not realize);

2. strong coupling between internal degrees of freedom (it leads to the additional displacement of frequencies and fast energy redistribution).

The typical behavior of the uncontrolled unimolecular system at high energy level is that deposited energy will break the weaker bond. Thus for selective dissociation of stronger bond we should control at oscillations frequency (to excite the system), and deposited energy should be concentrated in stronger bond. Additionally, control should be robust and effective when its intensity is small (arbitrarily small). The problem is complicated by the fact that control is scalar. These features makes the problem of selective dissociation nontrivial and interesting.

6. MODEL OF CONTROLLED SYSTEM

To describe the vibrations of HCN system we use following notations: $Z_i = 1 - e^{-\alpha_i R_i} \quad (i = 1, 2)$ are Morse variables, R_1 and R_2 are the displacements of length of the CN and CH bonds from their equilibrium values $R_{1,eq}$ and $R_{2,eq}$, P_1 and P_2 are the conjugate momenta corresponding to R_1 and R_2, m_1 and m_2 are reduced masses ($\frac{1}{m_1} = \frac{1}{M_C} + \frac{1}{M_N}$ and $\frac{1}{m_2} = \frac{1}{M_C} + \frac{1}{M_H}$, where M_C , M_N , M_H — atomic masses of corresponding atoms).

The full Hamiltonian of the HCN molecule in external laser field (**?**):

$$H = H_{mol} - d(R_1, R_2)U(t) \qquad (15)$$

where H_{mol} — molecular Hamiltonian, and the second component represents the laser-molecule interaction, $U(t)$ is the electric field amplitude (as a function of time t) — control. Linear 3-atomic molecule is modelled as two coupled Morse oscillators. The coupling terms are of two kinds: one is a model independent kinetic coupling term and the other describes coupling within the interaction in internal coordinates. Corresponding HCN molecular Hamiltonian:

$$H_{mol} = H_1 + H_2 + H_{12} \qquad (16)$$

with:

$$H_i = \frac{P_i^2}{2m_i} + V_i(R_i) \qquad i = 1, 2 \qquad (17)$$

which is composed of a kinetic energy term and a potential energy term $V_i(R_i)$ for bond i of the form:

$$V_i(R_i) = V_{i1}Z_i^2 + V_{i2}Z_i^3 + V_{i3}Z_i^4 \quad i = 1, 2 \quad (18)$$

Potential energy term (18) represents an effective potential for each bond (initially in ground, then in excited states). Expressions (17) can be called bond energies (but they are not invariants in uncontrolled system). The kinetic and potential coupling terms constitute Hamiltonian of bonds interaction:

$$H_{12} = -\frac{1}{M_C}P_1P_2 + V_{12}(R_1, R_2) \qquad (19)$$

where:

$$V_{12}(R_1, R_2) = V_1Z_1Z_2 + V_2Z_1^2Z_2 + V_3Z_1Z_2^2 \quad (20)$$

Dipole moment of molecule was chosen to simulate that of an instantaneous dipole:

$$d(R_1, R_2) = d_e(d(R_1) - d(R_2)) =$$

$$d_e((R_1+R_{1,eq})e^{-\alpha R_1} - (R_2+R_{2,eq})e^{-\alpha R_2}) \quad (21)$$

In this equation d_e is meaningful an "equilibrium charge" of bonds (so the product of this value on equilibrium bond length gives equilibrium value of dipole moment).

The system parameters fitting the first 40 stretching vibrational levels in the spectrum (with error 0.01%) can be found in (Smith et al, 1991).

Finally, full Hamiltonian can be rewritten as follows:

$$H = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} - \frac{1}{M_C}P_1P_2 + V_1(R_1) + V_2(R_2) +$$

$$+V_{12}(R_1, R_2) - d_e(d(R_1) - d(R_2))U(t) \qquad (22)$$

Substitution of (22) into Hamilton equations

$$\frac{\partial r}{\partial t} = \frac{\partial H}{\partial p} \qquad \frac{\partial p}{\partial t} = -\frac{\partial H}{\partial r}$$

gives the following equations of motion :

$$\dot{R}_1 = \frac{P_1}{m_1} - \frac{P_2}{M_C} \qquad \dot{R}_2 = \frac{P_2}{m_2} - \frac{P_1}{M_C}$$

$$\dot{P}_1 = -V_1'(R_1) - V_{12_1}'(R_1, R_2) - d_e d'(R_1)U(t)$$

$$\dot{P}_2 = -V_2'(R_2) - V_{12_2}'(R_1, R_2) + d_e d'(R_2)U(t)$$

where the dot denotes the time derivative while the prime denotes the derivative with respect to corresponding variable.

7. CONTROL ALGORITHM AND SIMULATION RESULTS

Problem of selective dissociation of strong bond is rather complicated and can not be satisfactorily solved by means of nonfeedback control (e.g. excitation on resonant frequency of strong bond or excitation with slowly changing frequency). For the solution of problem various methods of control theory can be used, such as optimal control (**?**) or method of reference model on energy (Chen et al, 1997). However, control functions, designed by these methods, have some defects, such as nonrobustness and complicated form (it makes difficult applications of such control in experiments). Broadly speaking, control function should have simple temporal and frequency structure, and, as was mentioned above, it should be robust and effective when control intensity is small (arbitrarily small).

We will apply the speed-gradient type method to the partial oscillator. Control provided by this method, looks like negative friction.

The natural control goal is to increase the energy of the partial oscillator corresponding to the strong bond (other bond is regarded as absent). In this case the goal is: $Q = \gamma(H_1^* - H_1)^2 \to 0$, where H_1^* — desired value of energy (sufficiently high), H_1 — current value of partial oscillator energy (sum of the potential and kinetic terms): $H_1 = \frac{P_1^2}{2m_1} + V_1(R_1)$, γ — coefficient. According to the speed-gradient method we calculate derivative of the goal function: $\dot{Q} = 2\gamma(H_1^* - H_1)(-\dot{H}_1) = 2\gamma(H_1^* - H_1)(-d'(R_1))\dot{R}_1U(t)$. We take into account that derivative of the dipole moment function is negative during the major part of time, so the driving force have the same sign with velocity. Disturbance from the other bond and its dynamic are neglected in this control method (but not in the dynamics of whole controlled system). We should also note that if the value of bond energy is sufficiently high, then system dynamics changes cardinally (for example, bond dissociation takes place). Thus, we can consider that value of bond energy is less than desired sufficiently high level within the framework of current model. Then, opposition of the signs of control and velocity is enough for decreasing of the goal function. Simplest control algorithms of such type have the form of negative friction (viscous or dry) in strong bond:

$$U = \gamma\dot{R}_1, \qquad \gamma < 0 \qquad (23)$$

or

$$U = \gamma sign(\dot{R}_1), \qquad \gamma < 0 \qquad (24)$$

Such control, obviously, injects energy in the strong bond. However, deposited energy can break weak bond because of energy redistribution or excitation of this bond. One of the possibilities to avoid this situation is to stabilize certain regimes of oscillations, providing coordinated dynamics of bonds. It is obvious that anti-phase regime provides convenient coordinated dynamics of bonds — if the system in the anti-phase regime and control looks like negative friction in strong bond (i. e. have the opposite sign with corresponding velocity), then excitation of strong bond and suppression of weak bond vibration take place simultaneously. Thus selective dissociation of strong bond takes place as a result of energy injection in the strong bond and neutralization of excess energy in the weak bond. It is important that such control supports anti-phase regime, hence if the system initially in this regime and control is of described type then selective

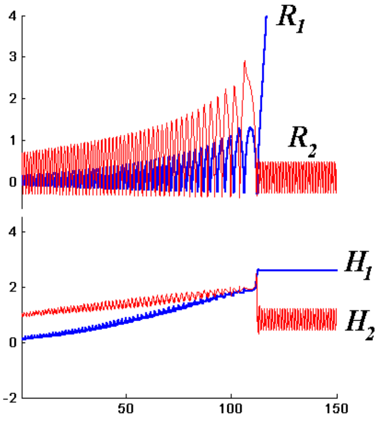

Fig. 2. Example of selective dissociation process.

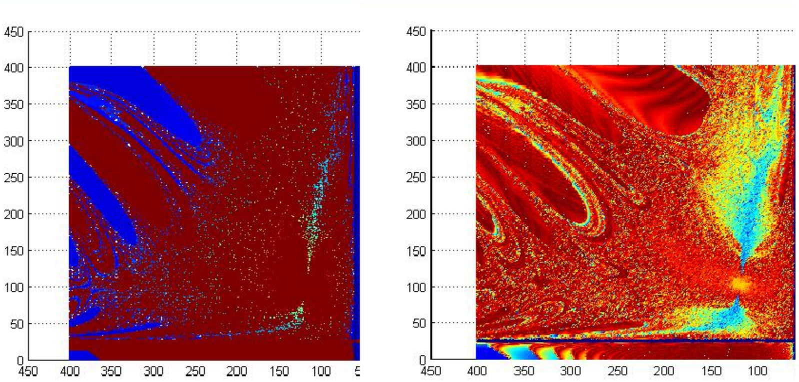

Fig. 3. Synchronization and selective dissociation.

dissociation of strong bond takes place almost surely. In Fig. 1 one can see an example of process, described above — system initially in the anti-phase regime, and control is given by (23) with $\gamma = -0.01$ (horizontal axis represents time, normalized on characteristic system period T_0 minimal period of the resonant oscillations in the linearized system).

One of the main advantages of this method is that if coefficient γ belongs to certain range $\gamma \in [\gamma_0, \gamma_1]$ then synchronization of oscillations in anti-phase regime takes place for initial data from rather wide region, and hence selective dissociation of strong bond takes place (according to the written above).

As an illustration of the connection between synchronization and selective dissociation one can see Fig. 2. For both pictures: control function is given by (23) with $\gamma = -0.01$, initial data — $(R_1, R_2, 0, 0)$ with $R_1, R_2 \in [1.54]$ (R_1 : horizontal axis, increasing from right to left; R_2 : vertical axis, increasing from bottom to top). For every initial data system with control is integrated during sufficiently long time. On the left picture : if selective dissociation of strong bond took place (strong bond dissociates, weak bond remains unbroken), then corresponding point of plane is painted over (color corresponds to time of dissociation : blue — minimum, brown — maximum). On the right picture : color of point corresponds to the index of synchronism Syn at the terminal moment (when dissociation of some bond occurs or time of integration comes to the end). Index of synchronism : $Syn = \frac{min(T_i,T_a)}{max(T_i,T_a)}$, where T_i, T_a are measures of time intervals when the system is oscillating synchronously, in in-phase and anti-phase mode, correspondingly. If the same point on both picture is painted close to blue, then selective dissociation of strong bond takes place after the synchronization in anti-phase regime.

8. CONCLUSIONS

In the paper the possibility of applying speed-gradient method to control of molecular systems is demonstrated for two problems: control of quantum observables for a diatomic molecule and dissociation control for a triatomic molecule with straight valence angle based on classical description of molecular dynamics. A substantial domain of initial conditions in the phase space of quantum system ensuring achievement of the control goal is determined both analytically and by means of computer simulation. An interesting observation is made that dissociation in a triatomic system often takes place after performing an anti-phase synchronous motion during some time.

REFERENCES

Ananjevsky, M., Efimov, A., Fradkov, A., Krivtsov, A. (2003) Resonance and speed-gradient design of control algorithms for dissociation of diatomic molecule ensembles. *Proc. 1st IEEE-IUTAM-EPS Conf. “Physics and Control”* St.Petersburg, pp. 867–878.

Brown E., Rabitz H. (2002) Some mathematical and algorithmic challenges in the control of quantum dynamics phenomena. *J. of Math. Chem.* V. 31, No. 1, pp. 17–63 .

Butkovsky, A.G., Samoilenko, Yu.I. (1980) *Control of quantum mechanical processes.* Dordrecht: Kluwer. (in Russian, 1984).

Chen, Yu., Gross, P., Ramakrishna, V., Rabitz, H., Mease, K., Singh, H. (1997) Control of Classical Regime Molecular Objectives - Applications of Tracking and Variations of the Theme. *Automatica.* V. 9, pp. 1617–1633.

Flugge, S. (1971) *Practical Quantum Mechanics 1.* Berlin-Heidelberg-New York: Springer-Verlag.

Fradkov, A.L., Miroshnik, I.V., Nikiforov, V.O. (1999) *Nonlinear and adaptive control of complex systems.* Dordrecht: Kluwer.

Krempl, S., Eisenhammer, T., Hubler, A., Mayer-Kress, G., Milloni, P. (1992) Optimal stimulation of a conservative nonlinear oscillator: classical and quantum-mechanical calculations. *Phys. Rev. Lett.* V. 69, No. 3, pp. 430–433.

Rice, S., Zhao, M. (2000) *Optical Control of Molecular Dynamics.* A Wiley-Interscience Publication.

Smith, A., Klemperer, W., Lehmann, K. (1991) *J. of Chem. Phys.* V. 94, 5040.