ANALYSIS OF CONTROLLED DISSOCIATION OF DIATOMIC MOLECULES BY THE METHOD OF MOLECULAR DYNAMICS

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During last decade a growing interest has been observed in the control problems for molecular systems in classical and quantum formulation [1-3]. One of the benchmark problems of that type is dissociation problem for diatomic molecule [2,3].

In this paper the two new methods for dissociation of diatomic molecule based on nonperiodic excitation generated by feedback control mechanism are proposed. The energy-feedback control uses frequency-energy (FE) relation of the natural oscillations to fulfill the resonance conditions at any time of excitation. The speed-gradient algorithm does not depend on the shape of the potential energy of molecule. Efficiency of the proposed methods is demonstrated by the problem of dissociation of hydrogen fluoride (HF) molecule. It is shown that new method is more efficient then methods based on constant frequency and linear chirping excitation.

The results of the paper extend those of the papers [4,5], in that an ensemble of molecules rather than single molecule has been studied based on the method of molecular dynamics.

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