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| Title: | Classical dynamics of molecules with quantum mechanical time dependent electronic forces |
| Authors: | Koner, A. |
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| Abstract: | The exact factorization method of Gross et al. is a complete solution of the molecular Hamiltonian in presence of a laser field. However, the method involves simultaneous solution of the electronic and nuclear parts and subsequently the time propagation of the full wavefunction; thus requiring large grid and hence is computationally expensive. An alternate methodology; which is approximate solves the electronic problem for fixed nuclear coordinates and involves time propagation of the electronic wavefunction in presence of laser. The nuclear dynamics is then carried out through classical dynamics in both the cases. The present work aims at identifying the set of conditions where the two methods give agreeable results and similar dynamics on an average scale for the model system of H_2^+ , where both of them can be applied. It should be noted that for models with larger degrees of freedom, only the approximate method coupled with classical dynamics is computationally feasible |
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