Quantum Dynamics with motions of large amplitude

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Many molecular processes, ranging from fundamental to applied problems, are known today to be impacted by strong nuclear quantum mechanical effects, including phenomena like tunneling, zero point energy effects, or non-adiabatic transitions. Recent success in helping to understand experimental observations in fields like heterogeneous catalysis, photochemistry, reactive scattering, optical spectroscopy, or femto- and attosecond chemistry and spectroscopy underlines that nuclear quantum mechanical effects affect many areas of chemical and physical research. The correct theory to describe the corresponding dynamics is Molecular Quantum Dynamics [1,2] . In contrast to standard quantum chemistry calculations, where the nuclei are treated classically, molecular quantum dynamics can cover quantum mechanical effects in their motion. New strategies have been developed successfully to extend the studies to systems of increasing size. In particular, we present here several applications in quantum dynamics mainly with the Multi-Configuration Time-Dependent Hartree method (MCTDH) developed in the group of Heidelberg [3,4] to the understanding and the control of molecular processes. MCTDH can be seen as a time-dependent MCSCF approach for the nuclei where wavepackets are propagated on one orseveral potential energy surfaces. Several examples, illustrating the flexibility of the approach, will bepresented involving a strong reorganizing of the atoms and thus motions of large amplitude [5] .

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