MCTDH CALCULATION OF INELASTIC COLLISION OF COMPLEX MOLECULAR SYSTEMS

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The details of energy transfer between colliding atoms and molecules is essential in order to understand chemical processes such as those in Earth's or other atmospheres, the Interstellar Medium (ISM) or for combustion chemistry processes in industrial and aeronautic applications. The most accurate and reliable data for these applications are mostly based on fully quantum mechanical calculations (classical treatments of the nuclei usually lead to inaccuracies, in particular when low temperature processes (common in the ISM) are of interest). To counter the curse-of-dimensionality (COD) problem that arises when cross-section calculations are performed on molecular systems with large masses (and thus dense state densities), two particularly promising methods have been developed recently: the Statistical Adiabatic Channel Model (SACM) and the Mixed Quantum-Classical Trajectory (MQCT) approach. We have also recently highlighted the effectiveness of the MultiConfiguration Time Dependent Hartree (MCTDH) approach to overcome the COD issue arising in the calculation of cross-sections of inelastic collisions. Indeed, since its inception, the MCTDH approach has allowed characterization, using a fully quantum dynamical approach and with an excellent accuracy, the spectroscopy and the dynamics for several challenging molecular systems and is thus known to push the boundaries of traditional quantum dynamical calculations. We will present our recent progress on this topic and discuss recent (and some preliminary) results on the collisions of H_2O with Ar, H_2 and H_2O using the MCTDH approach. We will also present the results of other collisions processes ($HCOOCH_3$+He, CH_3CH_2COH+He, N_2H^++H_2, ...) which remain challenging with standard computation approaches. We will also discuss the limitations of the approach and possible routes for improvements.