Time-dependent investigations of scattering processes

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Quantum mechanical calculations of reaction probabilities for atom-molecule collisions are calculated time-dependently with wavepackets. We want to investigate the dynamics on coupled PESs ($H + H_2^+$, $H^+ + H_2$ [1]; NeH_2^+, NeH_2 [2]). New results for the total angular momentum $J \neq 0$ will be presented. As a test reaction we use the $H + H_2$ (D_2) system [3]. The calculated state-to-state reaction probabilities using product-Jacobi-coordinates will be compared with energy resolved reaction probabilities calculated with the flux-operator using reactant-Jacobi-coordinates. Our aim is to produce accurate cross sections for the reactions mentioned above . For the $H + H_2$ reaction we compare the accurate results for several $J \neq 0$ values with different approaches (J-shifting and helicity decoupled calculations).

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