Wave packet calculations for ion-molecule reactions

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Quantum mechanical calculations of reaction probabilities for atom-molecule collisions are calculated time-dependently with wavepackets (using the Chebychev or split-operator method for propagation). Our aim is to perform the time-dependent treatment of collision dynamics on coupled PESs for the systems $H + H_2^+$, $H^+ + H_2$ [1]; NeH_2^+, NeH_2 [2]; H_3^-, H_3 [3].

New results for the reaction $Ne + H_2^+ \rightarrow NeH + H^+$ and $H^- + H_2$ will be presented. 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 and with time-independent calculations (NeH_2^+: [4]). The potential well of ca. 0.5 eV (NeH_2^+) leads to strong resonances in the reaction probabilities, showing a sensitive influence of the results on the input parameters, i.e. propagation time, grid size, etc. and allowing a critical comparison with the time-independent calculations.

In the case of $H^- + H_2$ and $H^- + D_2$ we will compare our results with experimental integral and differential cross sections. Further work is in progress for using filter-diagonalization techniques in order to make long propagation times superfluous.

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