Reactivity with transition states and angular momenta

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A transition state is a channel that connects in a dynamical sense two stable chemical states A and B. In dynamical terms states A and B are often stable equilibria, whereas the transition state (TS) is in close relationship with an unstable equilibrium. This unstable state is termed a *transition state* because, firstly, it is a bottleneck through which the density of probability that represent the dynamical state has to pass in order to transport the system from A to B, and secondly, because the TS itself is an unstable dynamical state that has observable physical manifestations and has to decay into either A or B as it evolves.

In this presentation, we wish to provide some descriptions and illustrations of unstable equilibria and TS as well as their dynamical usefulness and the simple ways they can be used in order to calculate reaction rates. We also focus on the various angular momenta that occur in reactive or inelastic scattering.

We illustrate the theory with specific examples relevant to molecular astrophysics [1, 2, 3]. In particular, the importance of angular momentum in reactive scattering will be underlined. At low energies, when centrifugal energy become comparable to asymptotic kinetic energy of the fragments the rate of energy transfer of the reaction rate between reactants becomes highly dependent on the TS and the dynamics associated with it.

References

[1] Alexandre Faure, Laurent Wiesenfeld, and Pierre Valiron, *Chemical Physics* 2000 254, 49.

[2] Laurent Wiesenfeld, Alexandre Faure, and Thomas Johann, *J. Phys B, At. Mol. Phys.*, 2003, 36 1319.

[3] Laurent Wiesenfeld, *Advances in Chemical Physics*, 2005, 130, 217.