Quantum trajectory capture at low temperature

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The classical capture model for chemical reactions assumes that all trajectories with enough energy to cross the (centrifugal) barrier in the effective potential actually do so, and then proceed to form the products. However, wave effects (not accounted for in a classical approach, by definition) become increasingly important with decreasing temperature and may dominate the collisional behavior at ultra-low temperatures.

In this contribution we propose a new approach that describes the capture process by evolving quantum trajectories [1,2] in the reactant channel up to a given limit, the *capture distance*, on the inside of the centrifugal barrier. The quantum trajectories take full account of quantum effects along the reaction path direction in the entrance channel. In particular, tunneling and quantum reflection, which can change the reaction rate by orders of magnitude, are accurately computed. In addition, quantum trajectories give valuable physical insight into the quantum capture process all along the approach of the reactants. They also provide a technical means to determine the optimum capture distance.

Moreover, quantum trajectories along the reactant approach can easily be coupled with classical trajectories that drive the rest of the degrees of freedom of the system [3]. Apart from the capture process, which is guided by a quantum trajectory, all other coordinates are treated classically [3]. This mixed quantum-classical capture approach is thus highly "classical-like" [3] and is aimed at large system reactions with quantum effects, still out of reach for current quantum scattering codes.

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2. *Quantum mechanics without wavefunctions*, J. Schiff and B. Poirier, *J. Chem. Phys.* **136**, 031102 (2012).
3. *Classical-like trajectory simulations for accurate computation of quantum reactive scattering probabilities*, G. Parlant, Y.-C. Ou, K. Park, and B. Poirier, *Comp. Theor. Chem.* **990**, 3 (2012).