Quantum trajectory capture for complex-forming reactions

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While direct reactions with activation barriers are now routinely calculated, reactions going through a long-lived intermediate complex are much more difficult to study[1, 2]. Complex-forming reactions are often barrierless and are thus relevant to the field of cold and utra-cold chemistry [2]. With decreasing temperature, wave effects become increasingly important and may dominate the collisional behavior at ultralow temperatures.

Capture theories (close-coupling expansion with boundary conditions applied in the reactant channel) are often used to study complex-forming reactions [3, 4]. In this contribution we propose a new approach that describes the capture process by evolving quantum trajectories in the reactant channel up to a given limit inside the centrifugal barrier. The quantum trajectories take full account of quantum effects [5] along the reaction path direction. In particular, tunneling effects, which can change the reaction rate by orders of magnitude, are accurately computed.

Apart from the entrance channel motion, which is guided by quantum trajectories, all other coordinates are treated classically [6]. Our trajectory method is thus highly "classical-like" [6]. It is aimed at large system reactions with quantum effects, still out of reach for current quantum scattering codes. Preliminary results will be presented at the conference.

References

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