A classical ride through a conical intersection

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Regarding the correlated electron-nuclear motion in a model system, we investigate the dynamics in the vicinity of a conical intersection (CoIn) between two excited state potential surfaces. It is documented that an ensemble of classical trajectories which move in the complete electronic-nuclear phase space tracks the quantum wave-packet motion through the CoIn which is accompanied by a strong non-adiabatic population transfer. On the contrary, for an adiabatic circular motion around the position of the CoIn, the quantum mechanical and classical densities deviate substantially. In the latter case, the Born-Oppenheimer classical nuclear motion on a single potential surface is able to track the quantum dynamics.

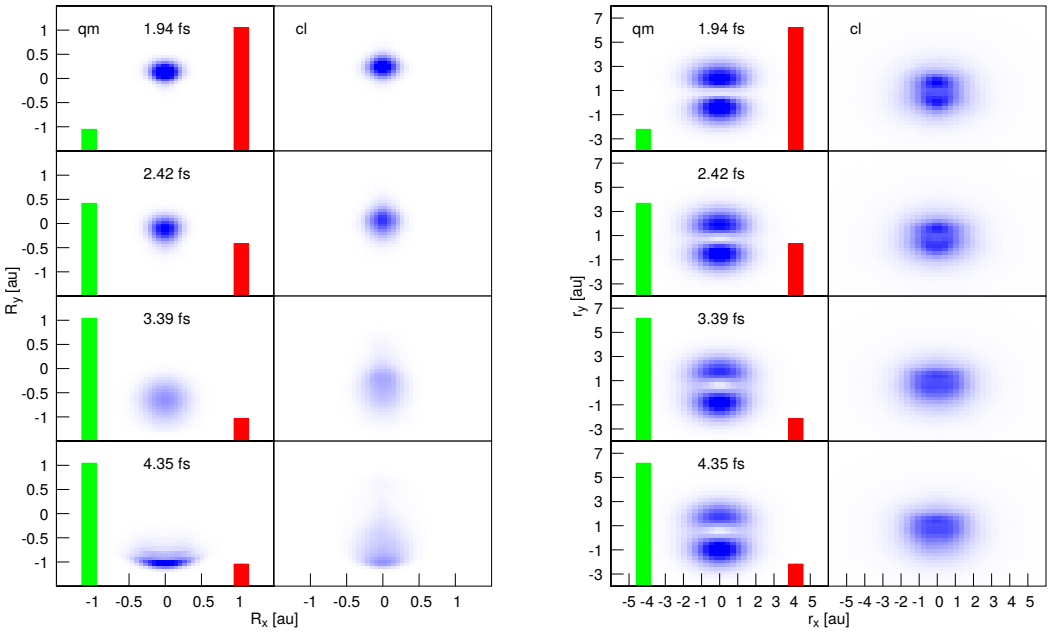

Figure 1: Quantum (qm) nuclear density, with its classical (cl) counterpart (left). Quantum electronic density and its classical counterpart (right). The bars show the population of the second (green) and first (red) excited state.

References

1. Schaupp T., Engel V., *J. Chem. Phys.* **150**, 034301 (2019)