

Prerequisites:

- Introduction of generalized coordinates
- KE energy operator in Lagrange form
- Analytical approximations for PES and IDS

Individual trajectory:

- Generate initial condition (MCMC)
- Scattering trajectory propagation
- FT of dipole time function

Collecting and post-processing:

- Spectral function as ensemble average
- Calculate spectral profile
- Desymmetrization

2-5 mln. trajectories

