Supplementary Material (ESI) for PCCP

Supplementary material

Trajectory-based solution of the nonadiabatic quantum dynamics equations: an on-the-fly approach for molecular dynamics simulations

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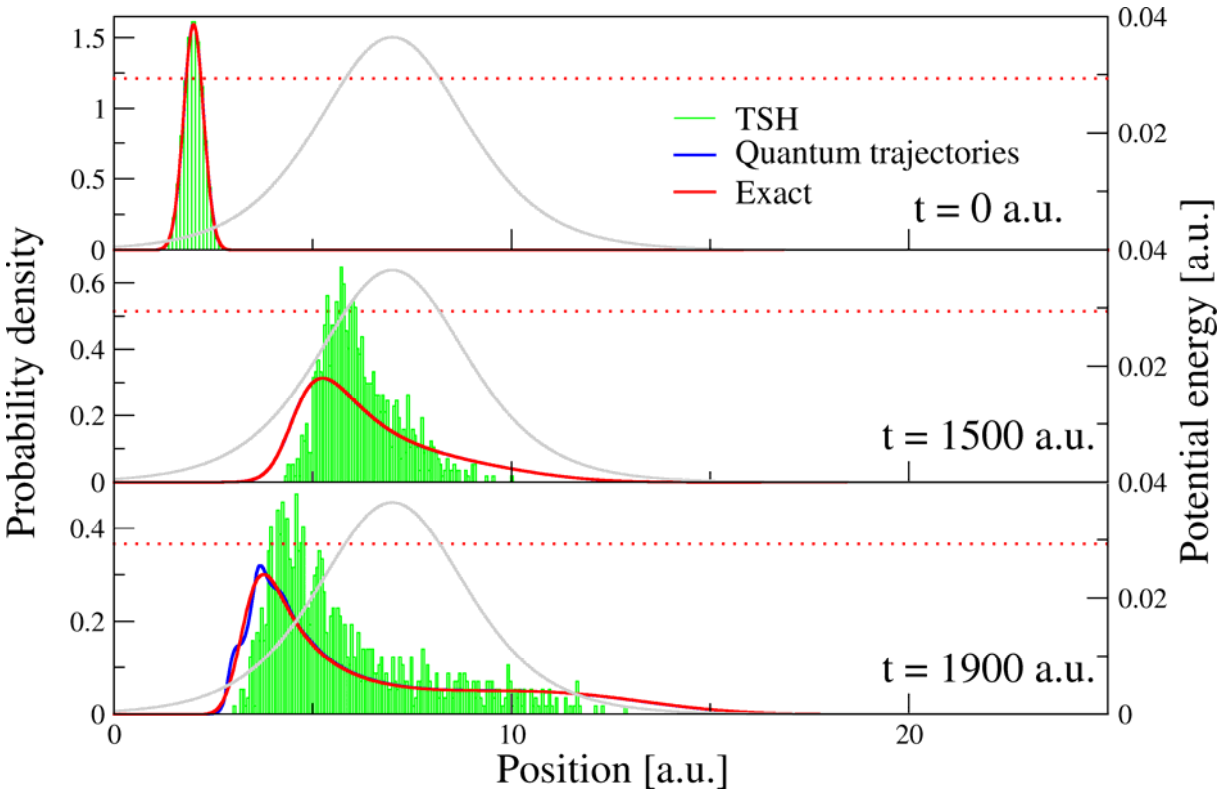

The figure shows three subsequent snapshots of a wavepacket (probability density) colliding with a 0.36 a.u. high Eckart potential centered at x=7 a.u.. The simulation was started with a Gaussian wavepacket centered at x=0 a.u. (kinetic energy 0.294 a.u. and initial momentum pointing to the right). Quantum trajectories can reproduce the exact dynamics of the wavepacket while TSH gives a larger wavepacket reflection due to the lack of tunneling.
See B. K. Kendrick , J. Chem. Phys., 2003, **119**, 5805–5817 for additional details related to the propagation of quantum trajectories for this system.