Chemical Dynamics

Elective course with a weekly load of two lectures 1.5 hours each. In addition to the syllabus below, this course will also serve as an introduction to numerical simulations using a high-level language like Python or Julia.

Syllabus

1. Introduction to time-dependent phenomena
    a. Time-dependent Schrodinger equation
    b. Born-Oppenheimer (BO) approximation as basis of molecular dynamics
    c. Break-down of BO approximation: conical intersections, non-adiabatic processes.
    d. Diagonal corrections to BO surfaces
    e. Full corrections to BO dynamics
2. Time evolution of wavepackets
    a. Gaussian wavepacket propagation under harmonic potentials
    b. Introduction to semiclassical ideas: Heller's thawed Gaussian dynamics
3. Time-dependent perturbation theory
    a. Interaction picture
    b. Fermi's Golden Rule
    c. Redfield approximation
4. Correlation functions
    a. Ensemble version of Fermi's Golden rule leads to correlation functions
    b. Connections to spectroscopy
    c. Quantum vs Classical correlation functions
    d. Corrections to classical correlation function to obtain quantum results.
5. Analysis of thermal correlation functions
    a. Eigen-state expansion, Density Matrices
    b. Requirement of Monte Carlo for thermal correlation functions
    c. Introduction to imaginary-time path integral for quantum thermodynamics
        i. Trotter splitting
        ii. Classical limit
    d. Ring polymer molecular dynamics: approximate estimation of quantum correlation function
    e. Connections with classical correlation functions.

References

1. M. E. Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation* (Oxford University Press, Oxford; New York, 2010).
2. E. J. Heller, *The Semiclassical Way to Dynamics and Spectroscopy* (Princeton University Press, 2018).

Prerequisites

Introduction to Quantum Mechanics; Mathematical Methods

Grading

This course will primarily be graded through weekly or fortnightly homework assignments. The assignments will also have a component of simulations.