

CH-453

Molecular quantum dynamics

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Cursus	Sem.	Type
Chemistry and Chemical Engineering		Obl.
Chimiste	MA2, MA4	Opt.
Computational science and Engineering	MA2, MA4	Opt.

Language of teaching	English
Credits	3
Session	Summer
Semester	Spring
Exam	Oral
Workload	90h
Weeks	14
Hours	3 weekly
Courses	2 weekly
Exercises	1 weekly
Number of positions	

Summary

The course covers several exact, approximate, and numerical methods to solve the time-dependent molecular Schrödinger equation, and applications including calculations of molecular electronic spectra. More advanced topics include introduction to the semiclassical methods and Feynman path integral.

Content

- Review of classical molecular dynamics.
Langrangian and Hamiltonian formalisms, phase space.
Classical molecular dynamics and thermodynamics in phase space.
- Exact real-time quantum dynamics.
Time-dependent Schrödinger's equation. Born-Oppenheimer approximation and potential energy surfaces.
Time-correlation functions.
Methods of quantum propagation of wave functions.
Split operator method and the fast Fourier transform.
- Approximate methods for quantum dynamics.
Sudden approximation.
Adiabatic approximation.
Time-dependant perturbation theory.
Fermi's Golden Rule.
Time-dependent Hartree method.
- Semiclassical dynamics.
Old quantum theory and the WKB approximation.
Wigner function.
Van Vleck propagator.
Semiclassical initial value representation.
- Quantum thermodynamics.
Feynman path integral approach
- interpreted as imaginary-time dynamics
- interpreted as classical thermodynamics of a polymer chain.
Path integral Monte Carlo method.
Path integral molecular dynamics.

Learning Outcomes

By the end of the course, the student must be able to:

- Solve the time-dependent Schrödinger equation with a basis method.
- Derive and apply the sudden and adiabatic approximations.
- Derive the time-dependent perturbation theory and Fermi's Golden Rule.
- Apply the time-dependent perturbation theory and Fermi's Golden Rule to molecular transitions induced by

electromagnetic field.

- Expound the connections between the Newtonian, Lagrangian, and Hamiltonian approaches to classical mechanics.
- Expound how electronic spectra can be computed via the autocorrelation functions.
- Apply the Fourier and split-operator methods to solve the time-dependent Schrödinger equation numerically.
- Expound the connection between quantum dynamics and quantum thermodynamics and how it can be used to compute molecular quantum thermodynamic properties with the Feynman path integral.

Assessment methods

Grade: 25% exercises during the semester; 75% oral exam

Supervision

Office hours	Yes
Assistants	Yes

Resources

Ressources en bibliothèque

- [Introduction to quantum mechanics / Tannor](#)
- [Quantum mechanics in chemistry / Schatz](#)

Websites

- http://scgc.epfl.ch/telechargement_cours_chimie