CH-453

Molecular quantum dynamics

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

Language of teaching	English
Credits	3
Session	Summer
Semester	Spring
Exam	During the semester
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

1. Review of classical molecular dynamics.
Langrangian and Hamiltonian formalisms, phase space.
Classical molecular dynamics and thermodynamics in phase space.
2. 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.
3. Approximate methods for quantum dynamics.
Sudden approximation.
Adiabatic approximation.
Time-dependant perturbation theory.
Fermi's Golden Rule.
Time-dependent Hartree method.
4. Semiclassical dynamics.
Old quantum theory and the WKB approximation.
Wigner function.
Van Vleck propagator.
Semiclassical initial value representation.
5. Quantum thermodynamics.
Feyman 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