

CH-453

**Molecular quantum dynamics**

Vanicek Jiri

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.
Chimiste	MA2, MA4	Opt.
Computational science and Engineering	MA2, MA4	Opt.
Minor in Quantum Science and Engineering	E	Opt.
Quantum Science and Engineering	MA2, MA4	Opt.

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

**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

#### Bibliography

- Quantum mechanics in chemistry / Schatz
- Introduction to quantum mechanics / Tannor

#### Ressources en bibliothèque

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

#### Websites

- [http://scgc.epfl.ch/telechargement\\_cours\\_chimie](http://scgc.epfl.ch/telechargement_cours_chimie)

#### Moodle Link

- <https://go.epfl.ch/CH-453>