



FBB3130 Quantum Dynamics

7.5 credits

Kvantdynamik

This is a translation of the Swedish, legally binding, course syllabus.

Establishment

Course syllabus for FBB3130 valid from Spring 2016

Grading scale

G

Education cycle

Third cycle

Specific prerequisites

- Three years at the School of Chemistry, Chemical Engineering and Biotechnology, KTH, or equivalent.
- Courses in Quantum Mechanics, Quantum Chemistry and Molecular Modeling are helpful.
- Some basic experience with computers.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

After a successful course completion, the student will be able:

- 1) to know general principles of different types of optical and X-ray spectroscopies;
- 2) to be able to use both dynamical and time-independent approaches in spectroscopy;
- 3) to know the meaning of the wave packet and to be able to solve time dependent Schrödinger equation for free propagation and harmonic potential;
- 4) to derive the Fermi-Golden rule and the rates of absorption, photoionization, emission and Auger processes;
- 5) to know how the X-ray ionization and absorption spectroscopies give the structure information;
- 6) to model resonant X-ray Raman and Auger scattering taking into account both electronic and nuclear degrees of freedom;
- 7) to model the interaction of molecules with strong electromagnetic field.

Course contents

A lecture course is focusing on spectroscopy and physics related to modern laser, synchrotron and X-ray free electron laser sources with chemical and biological applications. The course consists of 11 lectures and home exercises.

Lecture 1. Basic quantum mechanics. Schrödinger equation. Coordinate-time uncertainty principle. Spectrum: continuum and bound states. Hydrogen atom.

Lecture 2. Time-dependent perturbation theory. Fermi Golden Rule. Time-energy uncertainty principle and the problem related with this principle.

Lecture 3. Homogeneous and inhomogeneous broadening of spectral lines. Lifetime of excited state: Radiative versus Auger decay channels. Momentum and angular momentum conservation laws. Translational and rotational Doppler broadening. Translational and rotational recoil effects.

Lecture 4. Photoelectron spectroscopy: Chemical and Biological applications. Chemical shift of core-level. Born-Oppenheimer approximation. Vibrational and rotational structure. Translational and rotational Doppler effects. Young's double/multiple slit interference.

Lecture 5. Quantum dynamics. Wave packet of free motion and wave packet in harmonic potential.

Lecture 6. Optical and X-ray absorption spectroscopy of atoms and molecules. Applications. NEXAFS spectroscopy. Structure of the continuum wave function. EXAFS spectroscopy: structure determination of disordered systems.

Lecture 7. Coincidence spectroscopy as a tool to study fixed in space molecules.

Applications.

Lecture 8. Time-dependent theory of the light scattering. Resonant and non-resonant optical and X-ray Raman scattering. Resonant Auger spectroscopy.

Lecture 9. Dynamics versus interference. Lifetime vibrational and rotational interference. Scattering duration versus the detuning. Reversible and irreversible quenching of the wave packet of excited state.

Lecture 10. Applications of Raman and Auger spectroscopies.

Lecture 11. Stimulated emission and Lasing. Non-linear spectroscopy. Rabi solution and Rabi oscillations. X-ray free-electron laser and overview of its applications".

Course literature

1. Reinhard Schinke, Photodissociation Dynamics, Cambridge University Press, Cambridge, 1995.
2. Sune Svanberg, Atomic and Molecular Spectroscopy, Springer-Verlag, Heidelberg, 2001.

Examination

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

Oral examination with written preparation, which includes 2 theoretical questions and solution of 2 problems.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.