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 Autumn 2010

Grading scale

G

Education cycle

Third cycle

Specific prerequisites

Basic knowledge of Fortran is required since subroutines that calculate wave packet and pulse propagation are written in Fortran.

Background in quantum mechanics and electromagnetic field theory.

Language of instruction

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

Intended learning outcomes

"Quantum dynamics" (QD) provides a comprehensive theoretical tool of this multidisciplinary field, offering a wide range of problems covering: Background science, ultra-fast dynamics and structure of materials, dynamical aspects of different spectroscopies including absorption, emission, scattering and pulse propagation through resonant media as well as different technological applications.

"Quantum dynamics" introduces students to important and timely concepts and knowledge. This course is intended for students who wish to learn about quantum dynamics of molecular motion in external fields, as well as applications in different spectroscopies and non-linear optics.

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

1) Understand the fundamental principle of molecular dynamics on quantum level.

2) Compute and visualize dynamics of the wave packet and laser field. To get experience in quantum dynamical simulations and to understand the role of the time in different physical chemical processes in external fields.

3) Understand the dynamics of the molecules in electromagnetic field and propagation of the laser pulses through the resonant media and to get experience in quantum dynamical simulations.

Course contents

Quantum dynamics is the background of molecular and optical physics, which has impact in different fields, from molecular dynamics and light propagation to different

applications like quantum computing, molecular electronics and material sciences. The QD is the front page of modern physics and chemistry due to ultrashort laser infra-red and optical sciences pulses (from femtosecond to attosecond time domains). Femtosecond x-ray pulses are already available in FLASH (Hamburg) and Stanford Linear Accelerator Center. This new source of ultra-short x-ray pulses opens unique opportunity to map molecular dynamics with the Ångström resolution which of crucial importance in material sciences and biology.

"Quantum dynamics" gives students important concept of the dynamics of different physical chemical processes.

The course is intended for anyone who wishes to learn the current state of ultrafast phenomena in chemistry and physics.

This course has been developed in parallel with the fast-advancing multidisciplinary research and technological developments related to the ultrafast molecular dynamics, and addresses three main topics:

Part 1: fundamental quantum mechanics of light-matter interaction /quantum molecular dynamics and dynamics of light propagation

Part 2 time-dependent spectroscopies

Part 3: dynamics of propagation of ultra-short light pulses.

Lectures

1) Stationary Schrödinger equation. Born-Oppenheimer approximation. Electronic and nuclear degrees of freedom

2) Time-dependent Schrödinger equation. Harmonic oscillator. Dissociation.

3) General properties of the wave-packet: Quantum versus classical dynamics. Revival phenomenon

4) Dynamics of the Interaction between photons and molecules. Fermi Golden rule. Franck-Condon principle

5) Mechanisms of the relaxation of excited electronic state. Dynamics of photoabsorption and fluorescence. Mechanisms of the spectral line broadening.

6) Dynamics of the Raman scattering and Kramers-Heisenberg equation. Duration of the light scattering.

7) Numerical computations.

8) Dynamics of the molecules in strong laser field. Density matrix formalism and Maxwell's equations

9) Radiative damage. Multi-photon ionization and dissociation of molecules.

10) Dynamics of pulse propagation. Area theorem.

11) Self-seeded Stimulated Raman scattering.

Four-wave mixing. Slowdown and compression of the pulse. Numerical computations.

12) Time-resolved structure determination.

Disposition

Six lecture times (each times 2x45 min lectures) with home assignments (there will be a reading before lecture ca 1 day work load; and work load for each home assignment is ca 2 day); Two computational laborations (work load ca 2 days for each lab) will be coordinated based on practical problems in Quantum dynamics. Total work load is ca 23 days.

Course literature

Detailed lecture notes will be distributed.

Course books

1.R.Schinke, Photodissociation Dynamics, Cambridge University Press, Cambridge, 1995

2.S.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.

Other requirements for final grade

For the base 7,5-credit part.

Home assignments (including computational exercises) of about 30 hours will be required and the results will also affect the final grade.

Attendants are required to complete written examination directly related to the courses (mostly concerning fundamental knowledge about concepts in wave packet technique, light-matter interaction and pulse propagation).

Two computational laborations will be coordinated based on practical problems in Quantum Dynamics , which will affect the final grade. The two lab projects will be positioned approximately at 1/4 and 3/4 time of the course, aiming at assessing functioning knowledge.

Examination:

5 home assignments, 1,5 credits, grade scale: P, F

LAB1 - Laboratory Work, 1,0 credits, grade scale: P, F

LAB2 - Laboratory Work, 1,0,credits, grade scale: P,F

Written examination, 4,0 credits, grade scale: A, B, C, D, E, FX, F

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.