



# FBB3130 Kvantdynamik 7,5 hp

## Quantum Dynamics

När kurs inte längre ges har student möjlighet att examineras under ytterligare två läsår.

## Fastställande

Kursplan för FBB3130 gäller från och med VT15

## Betygsskala

## Utbildningsnivå

Forskarnivå

## Särskild behörighet

- 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.

## Undervisningspråk

Undervisningspråk anges i kurstillfällesinformationen i kurs- och programkatalogen.

## Lärandemål

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 Augerscattering taking into account both electronic and nuclear degrees of freedom;
- 7) to model the interaction of molecules with strong electromagnetic field.

## Kursinnehåll

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".

## Kurslitteratur

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

2. Sune Svanberg, Atomic and Molecular Spectroscopy, Springer-Verlag, Heidelberg, 2001.

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2. Sune Svanberg, Atomic and Molecular Spectroscopy, Springer-Verlag, Heidelberg, 2001.

## Examination

Examinator beslutar, baserat på rekommendation från KTH:s handläggare av stöd till studenter med funktionsnedsättning, om eventuell anpassad examination för studenter med dokumenterad, varaktig funktionsnedsättning.

Examinator får medge annan examinationsform vid omexamination av enstaka studenter.

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

## Etiskt förhållningssätt

- Vid grupparbete har alla i gruppen ansvar för gruppens arbete.
- Vid examination ska varje student ärligt redovisa hjälp som erhållits och källor som använts.
- Vid muntlig examination ska varje student kunna redogöra för hela uppgiften och hela lösningen.