2022-08-28

Course Syllabus

KD2360 Quantum Chemistry
Department of Chemistry
Fall Quarter 1 2022-2023

Course description

The course consists of two parts. The essential quantum mechanics that is required later is covered in the first part. The basic quantum mechanical principles and their applications to model systems once mentioned in the basic course are discussed in detail. Approximative methods are introduced. The interaction between electromagnetic radiation and molecules is discussed which then leads to the basic principles of various optical (such as infrared and Raman) spectroscopies.

Methods of quantum chemical calculations and their applications in chemistry and biochemistry are treated in the second part of the course. The Hartree-Fock method, its theoretical background and implementation but also post-Hartree-Fock methods and the density functional theory are described and discussed. Their application for calculating molecular properties such as energies, molecular geometries, vibrational spectra and features of chemical reactions is introduced and illustrated. This part of the course includes quantum-chemical calculation assignments where a modern quantum chemical software package is used for computing molecular properties and chemical reactions.

Intended learning outcomes

- **Part I.** Describe in detail the formalism of quantum mechanics, relate to and summarize the concepts of quantum mechanics in order to define, calculate and explain the behavior of quantum mechanical model systems.
- **Part II.** Describe, explain and apply basic quantum chemical theory for atomic and molecular many-electron systems to the computation of molecular properties, chemical reactivity and molecular spectroscopy.

Prerequisites

The course has originally been set up for the students that are currently in the Engineering Chemistry (CTKEM) program here at KTH. Hence, prerequisites in mathematics and in physics are commensurate to the formal content of the mathematics, physics, and physical chemistry courses during years 1-3 of that program. It is up to each participant to see to it that those prerequisites are mastered.

Course Setup

Teachers

Nanna H. List, nalist@kth.se

István Furó, 790 8592, furo@kth.se (Examiner)

Tore Brinck, 790 8210, tore@kth.se

We are located at the Department of Chemistry, Teknikringen 30, plan 6, Tillämpad fysikalisk kemi corridor.

The initial course part (NL, IF) concerns basic quantum mechanics and its applications to simple model systems. The second half of the course (TB) concentrates on approximative methods as applied in quantum chemical calculations. The second part of the course also includes two computer laboratories.

Home assignments

Several home assignments are going to be given are given during the course. Points given at the home assignment will provide bonus points at max 20 % of the total points at the exam. In addition, the lab reports are going to be requested and are evaluated as simple P/F.

Exam

The course exam focuses on the two intended learning outcomes

Grade E	The points thresholds (40 %) for each individual course outcome are passed.
Grade Fx	The points thresholds (40 %) for one individual course outcome is passed and for the other at least 30 % is passed.
Grade D	Total >50 %
Grade C	Total >60 %
Grade B	Total >70 %
Grade A	Total >80 %

Readings, materials and resources

The following textbooks are recommended:

1. J. Griffiths: Introduction to Quantum Mechanics, 2nd ed. or J. Griffiths and D. F. Schroeter: Introduction to Quantum Mechanics, 3rd ed. both by Cambridge Uni Press
2. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover, 1995.

Please AVOID at the "pirated" edition J. Griffiths: Introduction to Quantum Mechanics, 2nd ed. by Pearson (New International edition).

We also provide Additional reading. In some cases, that material is a help to understand concepts better and in some other cases it may broaden the horizon of the interested. You should be perfectly capable to decided which material is for which of those (sometimes overlapping) purposes.

Course schedule and recommended readings

Important: the lecture notes define the course content! The chapters of the book(s) listed below provide direct support/repetition/elaboration/explanation.

Griffiths-Schroeter, Introduction to Quantum Mechanics, 3rd ed. = GR
Szabo-Ostlund, Modern Quantum Chemistry = SO

KD2360 – Part I	
Lectures 1-2 Initial knee bends: why do we need quantum mechanics, how does it manifest itself, and beyond	GR Chapter 1 GR Ch 2.1-2 GR Ch 2.6 GR Ch 4.2.2 Although we do not mention most of the phenomena described there, GR Ch 12 may be an interesting read for some.
Lectures 3-4 Mathematical structure of quantum mechanics.	GR Ch 3 (except 3.4 after eq. 3.53) + Appendix Linear Algebra + Ch 2.4 pp 55-56
Lectures 5-6 Simple model systems of chemical relevance	GR Ch 2.3 GR Ch 4 (excl. 4.4)
Lecture 7 Introduction to spin and its consequences	GR Example 4.4 but without the rest of Ch 4.4.2. Not 4.4.3 or 4.5. GR Ch 5.1 GR Ch 5.2 (read as repetition/appetizer)
Lecture 8-9 An intro to perturbation theory, its time-dependent variant and how it relates to spectroscopies	GR Ch 11.1 – 11.4 GR Ch 11.3.3 (this is much narrower than the lecture note), plus some aspects of Ch 6 (scattered across the text)
Lecture 10	No corresponding chapter.
KD2360 – Part II	
Lecture 11 Introduction to quantum chemistry. The variational principle.	SO 1.3, 2.1.1 (alt GR 8.1)
Lecture 12 Linear variation functions. Approximate solutions for the H2+ molecule.	SO 1.3, 2.1.2 (alt GR 8.3)
Lecture 13 Introduction to many electron wavefunctions and the orbital approximation.	SO 2.1-2.2
Lecture 14 Energies and properties of orbital wavefunctions	SO 2.3, 3.1-3.3
Lecture 15	SO 3.4-3.5

Hartree-Fock method: theory and computational implementation. Basis sets for quantum chemical calculations.	
Lecture 16 Post Hartree-Fock + DFT methods. Analysis of chemical problems using quantum chemical methods.	SO 4.1-4.3, 4.6, 6.1 (Chapters are not covered in detail)
Lecture 17 Applications of Quantum Chemistry. Research at KTH and outside. Ideas Master projects.	No corresponding chapter

Computer laboratories

LI Hartree-Fock calculations: Geometry and rotational barrier of H_2O_2. Geometry and vibrational frequencies of acetamide.

L2 Studying chemical reactions by ab initio and DFT methods.