CHEM-UA 651: Quantum Mechanics and Spectroscopy

Semester: Spring, 2020
Professor: Mark E. Tuckerman
Office: 1166E Waverly
Office hours: Tuesdays 3:30 - 5:00 pm, 1001P Silver
Phone: 998-8471
E-mail: mark.tuckerman@nyu.edu

Basic Course Information

The text for the course is McQuarrie and Simons Physical Chemistry: A Molecular Approach. This book is required. A less technical overview of what we will be discussing this term can be found in the lighter but still fun recommended book Absolutely Small by Michael D. Fayer. A short but extremely useful treatment of quantum mechanics in chemistry is Ratner and Schatz Introduction to Quantum Mechanics in Chemistry.

Lectures are scheduled to meet from 2:00 pm to 3:15 am on Tuesdays and Thursdays in room 206 Silver.

Thursday recitation sections: 11:00 am to 12:15 pm in room 261 Meyer and 3:30 pm to 4:45 pm in room C-11 or the 25 W. 4th Street building.

Midterm exam dates: Midterm exam dates are scheduled for Locations will be announced when they are known.

Final exam date: The final exam is scheduled for Location will be announced.

Course content and math/physics background

The course will cover chapters 1-14 of the text, excluding chapters 2 and 11 (see attached course schedule). Topics include failures of classical mechanics, postulates of quantum mechanics, simple examples of the Schrödinger equation, quantum theory of electronic structure in atoms and molecules and the theory of the chemical bond, group theory, and molecular spectroscopy. Although the math and physics content is substantial, we will cover the topics needed in the course, including a set of preliminary lectures on the requisite mathematics. My opinion of the textbook is somewhat low, so when it serves a clear pedagogical purpose, I will stray from the book and make notes available to you on NYU classes.

Grading

The grading will be as follows: The midterms will count for 20% each, the final for another 20%, quizzes, 20% and homework 20%. Homeworks will be graded only for completeness. That is, if you make a sincere attempt to solve a problem, you will receive full credit for it, even if you do not get the right answer. However, you must get to a final answer to receive credit. Problems not attempted will receive no credit, and problems partially solved will receive partial credit not to exceed 50%.

Missed exams and quizzes

There will be no make-up midterm exams. You may make up one quiz over the course of the semester only if you have a valid, documented excuse for missing a quiz. The final can be made only if you have a valid, documented excuse for missing it. You will have to work around my schedule this summer (or next fall, if you are still at NYU) when arranging a time to make up the exam.
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Syllabus

Week 1: January 28, 30
   Introduction
   Math Chapter A: Complex numbers
   Math Chapter C: Vectors
   Math Chapters E & F: Matrices
   Problem set 1 given out on 1/30

Week 2: February 4, 6
   Math Chapters E & F: Matrices
   Math Chapter B: Probability and statistics
   Problem set 1 due on 2/4
   Problem set 2 given out on 2/4
   Quiz 1 at recitation

Week 3: February 11, 13
   Chapter 1: Introduction to quantum theory – failures of classical physics
   Chapter 4: Postulates of quantum mechanics and the Schrödinger equation
   Problem set 2 due on 2/13
   Problem set 3 given out on 2/13
   Quiz 2 at recitation

Week 4: February 18, 20
   Chapter 4: Postulates of quantum mechanics and the Schrödinger equation
   Chapter 3: Quantum particle in a box
   Problem set 3 due on 2/20
   Problem set 4 given out on 2/20
   Quiz 3 at recitation
**Week 5:** February 25, 27

- **Chapter 3:** Quantum particle in a box
- **Chapter 5:** Quantum harmonic oscillator
  - Problem set 4 due on 2/27
  - Quiz 4 at recitation

**Week 6:** March 3, 5

- **Chapter 5:** Quantum rigid rotator
- **Math Chapter D:** Spherical coordinates
  - Midterm 1 on weeks 1-5 given at recitations
  - Problem set 5 given out on 3/5

**Week 7:** March 10, 12

- **Chapter 6:** Exact quantum mechanics of the hydrogen atom
  - Problem set 5 due on 3/12
  - Problem set 6 given out on 3/12
  - Quiz 5 at recitation

**Week 8:** March 24, 26

- **Chapter 7:** The variational principle
- **Chapter 8:** Multielectron atoms
  - Problem set 6 due on 3/26
  - Problem set 7 given out on 3/26
  - Quiz 6 at recitation

**Week 9:** March 31, April 2

- **Chapter 9:** Chemical bonding in diatomic molecules: $\text{H}_2^+$ and the LCAO method
  - Problem set 7 due on 4/2
  - Problem set 8 given out on 4/2
  - Quiz 7 at recitation

**Week 10:** April 7, 9

- **Chapter 10:** Bonding in polyatomic molecules; rationalizing structure in organic chemistry
  - Problem set 8 due on 4/9
  - Quiz 8 at recitation

**Week 11:** April 14, 16

- **Chapter 12:** Introduction to group theory; point groups
Midterm 2 on weeks 6-10 given at recitations
Problem set 9 given out on 4/16

**Week 12**: April 21, 23

  - **Chapter 13**: Molecular spectroscopy
  - Problem set 9 due on 4/23
  - Problem set 10 given out on 4/23
  - Quiz 9 at recitation

**Week 13**: April 28, 30

  - **Chapter 13**: Molecular spectroscopy
  - **Chapter 14**: Nuclear magnetic resonance
  - Problem set 10 due on 4/30
  - Problem set 11 given out on 4/30
  - Quiz 10 at recitation

**Week 14**: May 5, 7

  - **Chapter 14**: Nuclear magnetic resonance
  - Problem set 11 due on 5/7
  - Quiz 11 at recitation

**Week 15-16**: May 13-19

  - **Final exam**: May 14, 2:00 - 3:50 pm. Location: TBA