Chemistry 271 - Fall 2006

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Dear Chem. 271 students,

Chem. 271 is a great class (if I do say so myself), in which you have an opportunity to learn an enormous amount. It is not an easy class. We are going to cover vast amounts of material rapidly. Everything is important. It builds on itself, and it prepares you for your future. You will be exposed to concepts and methods that you may not use immediately, but that are essential for understanding modern science.

Please notice that the class is scheduled for **1.5 hours per lecture**. We have one quarter to cover a great deal of material. I want to take a short break in the middle. I want to have time to answer questions. Also, I will miss a few classes. Therefore, I have reserved the **Chemistry Gazebo every Monday and Wednesday at 4:00 pm. Be prepared to attend extra classes a few times.** I will let you know ahead of time that we are having an extra class.

The lecture will be presented as Power Point slide shows. At least a few days prior to the lecture, the slides will be put on the web site as pdf files. These can be downloaded and printed. You can bring them to class and take notes on them. I strongly recommend that you do so. It will probably be impossible to copy everything that is shown fast enough to get it all down.

Teaching Assistants:

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Books

Required

***Elements of Quantum Mechanics*, Michael D. Fayer, Oxford, 2001**

Posted on the web site are Errata and Addenda. People from all over the world send me errors they find, and I put the fixes on the web. In addition, some topics that are not in the book are added in the Errata and Addenda, such as a derivation of Fermi's Golden Rule. Please make sure you look at the Errata and Addenda for each chapter because the book has mistakes.

Recommended (On reserve in the library, but you might want to buy.)

Pauling and Wilson - *Introduction to Quantum Mechanics*
(This is an inexpensive book that goes through a lot of basics in great detail.)
Cohen-Tannoudji, Diu, Laloe - *Quantum Mechanics,* Vols. I & II
(This is an expensive two-volume set that has everything. It will be a great reference for the rest of your life.)

Useful Quantum Mechanics

Pauling and Wilson - *Introduction to Quantum Mechanics*
Dirac - *The Principles of Quantum Mechanics*
Schiff - *Quantum Mechanics*
Bohm - *Quantum Mechanics*
Powell and Crasemann - *Quantum Mechanics*
Eyring, Walter, and Kimball - *Quantum Chemistry*
Messiah - *Quantum Mechanics,* Vols I & II

Useful Classical Mechanics

Goldstein - *Classical Mechanics*

Homework:

There will be approximately 10 homework sets during the class, about one per week. The problems are given below. Additional problems will be added as we go along. There are problems for each chapter except chapter 1. The problems are at the end of the book. Each problem set will cover 1 or 2 chapters. The problems will be due approximately the next lecture after the last of the material is covered in class. Therefore, you should do problems as soon as the material is covered in class. The due date for each problem set will be announced.

The problem sets will be collected and your grade will depend in part on the problem sets (see below).

PS #	Chapters Covered	Problems (**Chapter**:Problem #)
1	1-2	**2**:1-5
2	3-4	**3**:1,3-6; **4**:2-5
3	5	**5**:1,3-5
4	6	**6**:1-6
5	7-8	**7**:1-3; **8**:1,3
6	9-10	**9**:1-3,5; **10**:1
7	11-12	**11**:1,2; **12**:1,2
8	13-14	**13**:1,2; **14**:1,2
9	15-16	**15**:1-3; **16**:1-3
10	17	**17**:1,2

Test:

There will be a take home final. This test will be handed out about 10 days before the day the final is scheduled as listed in the "Time Schedule." For the final, you will be able to use books and notes. However, unlike the problem sets, you may not work with other people or discuss the final with anyone other than the class staff.

Guidelines for Homework:

The homework will be worth 40% of your grade. The homework will be checked for completeness and effort. It is not be corrected or graded for accuracy of the solutions. It will be given a grade. The grades will be 10, 5, and 0. A 10 will be given if you do everything and an inspection makes it clear that you have made a serious effort to do everything right. A 5 will be given if you do most of the problem set and have made a serious effort. A 0 will be given if you turn in something, but there is not much there or you don't turn in anything. The homework problem sets are not tests. You may work together. There will be numerous TA office hours where you can get help with the problems. Everyone should get all 40% on the homework.

To get full credit, it is necessary to use the following rules so that we can see what you have done. These rules also apply to the final exam.

1. Make it NEAT! If we can't read it, we can't grade it.
Recopy your answers, if necessary.

2. Write on <u>one</u> side of the page.

3. Maintain a logical order.
a. Number equations if you need to refer to them later.
b. Number pages.
c. Indicate problem number and part (*e.g.*, 2b) you are working on <u>at the top of each page</u>.
d. Explain steps (*i.e.*, say what you are doing).
e. Start each problem on a new page.

4. Note and explain any assumptions made.

5. Box and label important intermediate results and the final result.

6. Bind or staple everything together in order.

7. When the homework is returned, the answers will be posted on the Chem. 271 web site. You should go over your answers, comparing them to the posted solutions. This is a very important part of your learning in the course. Making a mistake on a problem set is OK if you then find out the correct way to do the problem from the posted solutions.

Grades:

The grading for this course is straightforward. The problem sets are worth 40% of the grade; the final is worth 60% of the grade. As discussed above, the problems sets are graded for completeness and effort, not for having everything perfectly correct. Everyone should get the full 40% on their problem sets. Ask for help from the TAs or your friends. The final will be graded for accuracy. Substantial partial credit will be given. This is a graduate course. I hope and expect to give everyone a good grade. The number one way to get a bad grade is to not do the work and not make a serious effort on the final. If you do everything, all of the problems in the problem sets and all of the final problems, you will almost certainly get a good grade.

Topics

Chapter 1 - Absolute Size and the Superposition Principle
Chapter 2 - Kets, Bras, Operators, and the Eigenvalue Problem
- A. Kets and Bras
- B. Linear Operators
- C. Eigenvalues and Eigenvectors

Chapter 3 - Momentum of a Free Particle and Wave Packets
- A. Momentum States of a Free Particle
- B. Normalization of the Momentum Eigenfunctions
- C. Wave Packets
- D. Wave Packet Motion and Group Velocities

Chapter 4 - Commutators, Dirac's Quantum Condition, and the Uncertainty Principle
- A. Dirac's Quantum Condition
- B. Commutators and Simultaneous Eigenfunctions
- C. Expectation Values and Averages
- D. The Uncertainty Principle

Chapter 5 - The Schrödinger Equation, Time Dependent and Time Independent
- A. The Schrödinger Equation
- B. The Equation of Motion of the Expectation Value
- C. The Free Particle Energy Eigenvalue Problem
- D. The Particle in a Box Energy Eigenvalue Problem
- E. Particle in a Finite Box, Tunneling and Ionization

Chapter 6 - The Harmonic Oscillator in the Schrödinger and Dirac Representations
- A. The Quantum Harmonic Oscillator in the Schrödinger Representation
- B. The Quantum Harmonic Oscillator in the Dirac Representation
- C. Time Dependent Harmonic Oscillator Wave Packet

Chapter 7 - The Hydrogen Atom
- A. Separation of the Schrödinger Equation
- B. Solutions of the Three One Dimensional Equations
- C. The Hydrogen Atom Wavefunctions

Chapter 8 - Time Dependent Two State Problem
- A. Electronic Excitation Transfer
- B. Projection Operators
- C. Stationary States
- D. The Non-degenerate Case and the Role of Thermal Fluctuations
- E. An Infinite System – Excitons

Chapter 9 - Perturbation Theory
- A. Perturbation Theory for Non-degenerate States

C. Antisymmetrization and the Pauli Principle
D. Singlet and Triplet States

Chapter 17 - The Covalent Bond

A. Separation of Electronic and Nuclear Motion: The Born-Oppenheimer Approximation
B. The Hydrogen Molecule Ion
C. The Hydrogen Molecule

Books in Chem. Library:

AUTHOR	TITLE	CALL NUMBER
Biedenharn, L.C.	Quantum Theory of Angular Momentum	QC174.1; B46; c. 3; SWAIN
Bohm, David	Quantum Theory	QC174.1; B6; c.15; PERM RES
Dirac, Paul	Lectures on Quantum Mechanics	QC174.1; D5; c.2; SWAIN
Dirac, Paul	Quantum Mechanics	AC174.2; D5; c.9; PERM RES
Eyring, Henry	Quantum Chemistry	QD453; E9; c.10; PERM RES
Hameka, H.F.	Introduction to Quantum Theory	QC174.1; H36; SWAIN
Jackson, J.D.	Mathematics for Quantum Mechanics	QA37; J18; SWAIN
Kauzmann, W.	Quantum Chemistry	539.2; K21; SWAIN
Lowdin, Per-Olov	Quantum Theory of Atoms, Molecules, and the Solid State	QC174; 1L6; c.5; SWAIN
Matthews, P.T.	Introduction to Quantum Mechanics	QC174.1; M34; c.2; SWAIN
Messiah, Albert	Quantum Mechanics, v. 1-2	QC174.1; M413; c. 10 (v.1)
Pauling & Wilson	Introduction to Quantum Mechanics	QC174.12; P38; c.14; PERM RES
Pitzer, Kenneth S.	Quantum Chemistry	QC174.1; P48; c. 1,4; SWAIN
Saxon, D.S.	Elementary Quantum Mechanics	QC174.1; S289; c.2; SWAIN
Schiff	Quantum Mechanics	QC174.12; S34; c.13; SWAIN
Sherwin, Chalmers	Introduction to Quantum Mechanics	QC174.1; S47; c.4; SWAIN