Chemistry 120A: Spring Semester, 2019
Organizational Information

(1) Instructor:

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(2) Textbook.

The required textbook is a good solid introduction to our class's main topics:
P.W.Atkins and R.S.Friedman, "Molecular Quantum Mechanics"
If you are after alternative presentations, then there are numerous good books available. A few to get you started include the following:
D.A.McQuarrie & J.D.Simon, "Physical Chemistry: A Molecular Approach"
P.W. Landshoff, A. Metherell, G. Rees "Essential Quantum Physics"
T.Engel, "Quantum Chemistry and Molecular Spectroscopy"
If your overcommitted professor can manage it, I will also post extensive notes on bcourses that may someday become a book…

(3) Class goals

You are going to learn 3 main things from this course, if all goes well.

I) You will learn the guts of quantum mechanics, the theory that describes matter (molecules!) at the atomic level. Every chemist, biologist and engineer will benefit from understanding this material.

II) You'll learn about the important idealized models built from exact quantum mechanics that can be used to understand spectroscopy, including microwave, infrared, UV/vis, and maybe others.

III) You will get a glimpse of the approximations to exact quantum mechanics that can be solved by computer to describe and in fact predict what the electrons are doing in molecules. This is why quantum mechanics is *relevant* to almost all areas of modern chemistry and allied fields.

My hope is that you will find this course both challenging and rewarding.

(4) Assessment

Problem sets	20%
2 mid-term exams	2 x 20%
Final exam	40%

1. Introduction to quantum mechanics

    W 1/23: Experiments showing the need for QM and wave review
    F 1/25: Free particle, wavepackets and motivation of quantum mechanics

2. Eigenvalue problems and quantization

    M 1/28: Particle in a box and form of the Schrodinger equation
    W 1/30: Fundamentals of state space
    F 2/1: Introduction to operators, Hermitian operators and eigenvalue problems

3. Postulates of quantum mechanics

    M 2/4: Postulates of quantum mechanics
    W 2/6: Basic physical implications
    F 2/8: Commuting observables and uncertainty principle

4. 2-Level system and the harmonic oscillator

    M 2/11: Two-level system: examples, exact treatment and perturbations
    W 2/13: Time-dependence of two level system
    F 2/15: Harmonic oscillator: Introduction and energy levels.

5. Harmonic oscillator, continued (mid-term 1)

    M 2/18: Academic holiday – no class.
    W 2/20: Exam review lecture
    F 2/22: Harmonic oscillator eigenfunctions. Applications.

6. Angular momentum and the hydrogen atom

    M 2/25: The rigid rotor and angular momentum
    W 2/27: Quantization of angular momentum
    F 3/1: Hydrogen atom energy levels and atomic orbitals

7. Approximation Methods

    M 3/4: Variational method – linear and non-linear.
    W 3/6: Time-independent perturbation theory for non-degenerate states
    F 3/8: Completing perturbation theory through second order.

8. Selection rules and spectroscopy

   M 3/11: Rotational (microwave) spectroscopy
   W 3/13: Vibrational frequencies and IR spectroscopy: diatomics
   F 3/15: Vibrational spectroscopy of polyatomics

9. Spin and many-electron atoms (mid-term 2)

   M 3/18: Review lecture for mid-term 2.
   W 3/20: Electron spin, Fermi statistics and determinants
   F 3/22: Helium atom in singlet and triplet states

10. Electrons in molecules

   M 4/1: Born-Oppenheimer approximation; electronic Schrodinger equation
   W 4/3: H2+, H2 and the 1- and 2-electron chemical bonds
   F 4/5: Huckel theory for pi electrons in conjugated molecules

11. Molecular orbital theory

   M 4/8: Hartree-Fock wavefunction, self-consistent field theory
   W 4/10: Molecular orbitals in molecules; photoelectron spectroscopy
   F 4/12: HF forces, and molecular properties.

12. Density functional theory

   M 4/15: Hohenberg-Kohn theorems & Kohn-Sham theory
   W 4/17: What is in a density functional?
   F 4/19: Modern DFT

13. Intermolecular interactions

   M 4/22: Permanent and induced electrostatics
   W 4/24: Perturbation theory and dispersion interactions
   F 4/26: Orbital interactions.

14. Excited states and electronic spectroscopy

   M 4/29: Wavefunctions for excited states
   W 5/1: Selection rules and electronic spectroscopy
   F 5/3: Vertical vs adiabatic transitions and Franck-Condon analysis.