Chem 3502/4502 **Physical Chemistry II (Quantum Mechanics)** 3 Credits

Spring Semester 2006

Prerequisites: One prior year chemistry, one prior year physics, one prior year calculus.

Time and Location: MWF 10:10 – 11:00, 331 Smith Hall.

Instructor: Chris Cramer (215 Smith Hall, 624-0859, cramer@chem.umn.edu).

TAs: Kin-Yiu Wong (101H Smith, 625-2909, kywong@chem.umn.edu)
George Giambasu (P176 Kolthoff, 625-6317, giambasu@chem.umn.edu)

Office Hours: CC: Tu 11:00-12:00, F 2:00-3:00
K-YW: Th 4:00-5:00, F 4:00-5:00
GG: Tu 2:00-4:00

Textbook: There is no required textbook. Daily class lectures will be distributed on the class website as pdf files. An *optional* book available in the bookstore is Engel, *Quantum Chemistry and Spectroscopy*, Pearson Benjamin Cummings, 2006.

Class Website: http://pollux.chem.umn.edu/~cramer/3502 -- site will include at a minimum all class materials. Note that you are welcome to use the upper division microcomputer lab in 176 Kolthoff Hall if you want to print class materials free of charge.

Coursework: The class is lecture-like in format, with the anticipated topics to be covered outlined below. Students are expected to keep up with posted class readings (they'll be made available at least a few days in advance) and to work on assigned homework problems (see below). My intent is to spend the first 5 to 10 minutes of each lecture going over a previously assigned problem, and the remainder on lecture/demonstration of new material. Classroom attendance is not required, but you are likely to have a ***much*** more difficult time if you fail to attend classes.

Homework: At the end of each day's lecture notes will be 2 homework problems. I will discuss the solution to the *first* of the problems at the start of the following lecture. Students should do the problem but will not be expected to turn in their work or solutions. The *second* homework problem, on the other hand, should be prepared to be turned in for grading. Each Friday, at the start of class, the solutions to all *second* homework problems will be collected. One of these, selected at random, will be graded carefully, while the other(s) will be more cursorily checked. Answer keys will be provided online after the graded homework is collected. ***As a result, no homework will be accepted after the class period in which it is due.***

Exams: Exams will be cumulative on all class materials up to that point, with heavy emphasis on new material covered since any prior exam. The final exam will cover the entire semester, with some additional emphasis on topics covered in the last two weeks of class (for which no in-term exam is scheduled). The format of the exams will combine multiple choice with one or two short problems chosen to have close correspondence to assigned homework. Arriving at the answer to either type of problem may well involve some mathematical calculations; space and relevant formulae required to perform such calculations will be provided. Exams will likely be given in two rooms. Room assignments will be announced in class. The exams will emphasize *conceptual* details over mathematical manipulations, but testing on a certain amount of the latter cannot be avoided. The final exam is 10:30-12:30, Wed., May 10. ***Under no conditions will it be possible to reschedule the final exam, nor can that exam somehow be dropped.***

Grading: There will be 4 exams during the semester and a final exam (see schedule below). Your lowest score will be dropped and the remaining 3 in-term exams will constitute 60% of your final grade. Graded homework will count for 10%, and the final exam will constitute the remaining 30% of your final grade. If you miss an exam, for whatever reason, the missed exam will be the dropped exam. If, through outrageous fortune, you are forced to miss *two* exams, we can discuss remedies at the appropriate time. ***Under no conditions will it be possible to reschedule the final exam, nor can that exam somehow be dropped***. The class will be graded on an **absolute scale**: The total number of possible points in the course is 500, and you must earn at least 400 points for an A–, 350 points for a B–, 275 points for a C–, and 250 points for a D. Thus, earning approximately 80% of possible points enters the A range, 70% the B range, 55% the C range, 50% the D range, and earning less than 50% of possible points will result in a failing grade. As warranted, "+" and "–" grades will be awarded within each range (typically the top and bottom one or two percent).

Calculators: No calculators, nor any other electronic devices, will be allowed during exams. You will be provided with all formulae required to solve problems (e.g., solutions to non-trivial integrals) and answers will be expressed in terms of constants that need not be reduced to decimal values.

Preparing for Exams: There is no free lunch. The most effective method to prepare for an exam is to study the lecture notes, the assigned problems, and prior exams (which can be found on the website). I am happy to discuss any of these items during office hours, as are the TAs, if you need feedback.

Academic Misconduct: I rigorously adhere to the IT policy on scholastic conduct. Cheating is morally repugnant. Graded homework problems should be worked on *alone* although collaboration on the homework problem to be discussed in class each day is encouraged for those who find group work instructive. We will proctor exams and take other steps to prevent copying. However, we first and foremost rely on your intrinsic personal integrity to avoid cheating.

CJC

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COURSE OUTLINE

Date	Topic/Reading
01/18	Discussion of Syllabus. Research presentation: What's Quantum Chemistry Good For?
01/20	Origins of quantum hypothesis, blackbody radiation, photoelectric effect, hydrogen atom line spectra. Philosophical environment of science at time.
01/23	One-electron atomic model. Wave-particle duality. the de Broglie wavelength.
01/25	The Schrödinger wave equation. Probability and quantum mechanics. Collapse of the wave function upon sampling.
01/27	Matrix and vector interpretation of wave functions and operators. Key linear algebraic details associated with quantum mechanics. Complex numbers. Dirac notation. The turnover rule. **Homework 1 due.**
01/30	Stationary states. Operators and their expectation values. The Uncertainty principle.
02/01	Free particles and the particle in a box.
02/03	Spectroscopy of the particle in a box. Parity. Selection rules. QM tunneling out of a box with one wall of finite height and width. **Homework 2 due.**
02/06	Exam I
02/08	The QM harmonic oscillator (guest lecturer: Professor David Blank).
02/10	The QM harmonic oscillator continued. Zero-point energy. Infrared spectroscopy.
02/13	Angular momentum, classical and QM. Polar coordinates. Raising and lowering operators. Eigenvalues of L_z and L^2.
02/15	Angular momentum eigenfunctions. The spherical harmonics.
02/17	Spectroscopy of the rigid rotator. Diffuse interstellar bands. **Homework 3 due.**
02/20	The QM hydrogen atom.
02/22	Hydrogenic orbitals.
02/24	Spectroscopy of the hydrogen atom. Electron spin. Spin-orbit coupling. The Zeeman effect. Electron-spin resonance spectroscopy. **Homework 4 due.**
02/27	Exam II

03/01	The variational principle. The Born-Oppenheimer approximation. Basis functions.
03/03	Examples of variational calculations. The helium atom.
03/06	More variational calculations. The hydrogen atom. Gaussian basis sets.
03/08	Antisymmetry. Fermions and bosons. Spin.
03/10	Two-electron wave functions. Hartree products. The Slater determinant. Many-electron wave functions. Spin orbitals. **Homework 5 due.**
03/20	Spin algebra. Singlet and triplet states. The Helium atom revisited.
03/22	Perturbation theory. Applications of perturbation theory.
03/24	Catch-up and review. **Homework 6 due.**
03/27	Exam III
03/29	Recap of variational principle and LCAO approach. Solution of the secular equation. (guest lecturer: Professor Sandy Lipsky)
03/31	Effective Hamiltonians. Hückel theory.
04/03	Recap of antisymmetry and Slater determinants. The Hartree-Fock self-consistent field method.
04/05	More HF formalism.
04/07	Water at the HF level. **Homework 7 due.**
04/10	Water continued.
04/12	Still more water (who knew it could be so interesting?)
04/14	Yet again… water. Koopmans' theorem. Geometry optimization. **Homework 8 due.**
04/17	Water, and another molecule too! Catch-up and review.
04/19	Exam IV
04/21	IT Day -- no class
04/24	The potential energy surface. Chemical equilibria and kinetics. Molecular QMHO approximation.
04/26	Infrared vibrational spectroscopy. Matrix isolation of reactive intermediates.
04/28	Quantum statistical mechanics and thermodynamics. **Homework 9 due.**
05/01	Electron correlation. Configuration interaction (CI).
05/03	Configuration interaction and Møller-Plesset perturbation theory.
05/05	Research Talk: Survey of Modern Uses of Molecular Quantum Mechanics. **Homework 10 due.**
05/10	Final exam, 10:30 AM