<u>Chemistry 8552</u>   **Quantum Mechanics II, sec 001**   <u>4 Credits</u>
Spring Semester 2018

Prerequisites: Undergrad physical chemistry courses, calculus, Chemistry 8551.

Time and Location: 2:30PM- 3:50PM MW (01/17/2018-05/04/2018), Smith Hall 121

Instructor: Laura Gagliardi (229 Smith Hall, 625-8299, gagliard@umn.edu)

TA: None

Office Hours: to be arranged directly with the instructor

Textbook: There is no required textbook. Daily class lectures will be distributed on the class website as pdf files. O*ptional* books available in the library:
  1) Molecular Electronic-Structure Theory by Trygve Helgaker, Poul Jorgensen and Jeppe Olsen, Ed. Wiley 2000.
  2) European Summerschool in Quantum Chemistry Book I, II, III Björn O. Roos and Per-Olof Widmark, Eds.
  3) Density Functional Theory An Advanced Course Eberhard Engel · Reiner M. Dreizler Springer-Verlag Berlin Heidelberg 2011.

Class Website: www.chem.umn.edu/groups/gagliardi
Site will include at a minimum all class materials. Note that you are welcome to use the upper division microcomputer lab 101D Smith Hall if you want to print class materials free of charge.

Coursework: The class is mainly lecture-like in format, with the anticipated topics to be covered outlined below. Students are expected to keep up with posted class readings and to work on assigned homework problems (see below). Classroom attendance is not required, but you are likely to have a ***much*** more difficult time if you fail to attend classes.

Some of the lectures will be taught in an experimental style emphasizing class discussion. Students should prepare for these lectures accordingly. The material to be emphasized in each class will be announced beforehand, for example, at the previous lecture.

Homework: At the end of some lectures some homework problems will be assigned. The problems should be turned in at the start of the following lecture. The solution to the problems will also be discussed at the start of the following lecture. Students should be prepared to participate actively into the discussion. Homework also consists of preparing for class discussion of the readings. Homework may be done in groups, if desired.

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 consists of writing

a Hartree-Fock code that will be presented by the students at the end of the course. Details will be given during the course.

Grading: There will be **two** in-term exams during the semester and the final consists of writing computer code (the details will be discussed during the class). The two in-term exams will constitute 30% of your final grade. Graded homework will count for 10%. The presentation and participation into the discussion will constitute 30%. The final exam will constitute the remaining 30% of your final grade. If you miss an exam, for whatever reason, we can discuss remedies at the appropriate time. 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 450 points for an A–, 350 points for a B–, 275 points for a C–, and 250 points for a D. Thus, earning approximately 90% 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).

Preparing for Exams: The most effective method to prepare for an exam is to study the lecture notes, the assigned problems, and the textbook and start writing the code already at the beginning of the course. I am happy to discuss any of these items during office hours, if you need feedback.

Academic Misconduct: I rigorously adhere to the CSE policy on scholastic conduct. Cheating is morally repugnant. 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.

Laura Gagliardi

COURSE OUTLINE

Date	Topic/Reading
Week 1	
W 01/17	NO LECTURE (It will be rescheduled)
Week 2	
M 01/22	L1 &L2 Elementary quantum chemistry: the Hartree Product; the Slater Determinant; He atom 2 electrons in 2 orbitals
W 01/24	L3 Coulomb and Exchange Integrals. The Hartree-Fock Method L4 A Hartree-Fock calculation on the water molecule
Week 3	
M 01/29	Discussion about computer project
W 02/31	NO LECTURE (RESCHEDULED)
Week 4	
M 02/05	L3 Second quantization: products of operators
W 02/07	L4 Density matrices; commutators and anticommutators; review of density functions and density matrices
Week 5	
M 02/12	Discussion 1
W 02/14	L5 Nonorthogonal spin orbitals; spin in second quantization: spin function operators in the orbital basis; spin tensor operators; spin properties of determinants Spin in second quantization: configuration state functions
Week 6	
M 02/19	L6 Orbital rotations: unitary transformations and matrix exponentials; unitary spin-orbital transformations; symmetry-restricted unitary transformations
W 02/21	L11 Discussion 2 L7 Exact and approximate wave functions: the exact wave function; the variational principle; size-extensivity
Week 7	
M 02/26	L8 Standard Models One- and N-electron expansions L9 Short-Range Interactions and Orbital Expansions: the Coulomb hole; the Coulomb cusp; approximate treatments of the ground-state helium atom
W 02/28	**Exam 1**
Week 8	

M 03/05	L13 Electron Correlation; H_2 in a minimal basis
W 03/07	L14 Configuration-Interaction Theory CASSCF and RASSCF; Size-extensivity and CI methods L15 CI: Slater determinants as products of alpha and beta strings; Direct CI methods
03/12-03/16	**SPRING BREAK**
Week 9	
M 03/19	L15 Discussion 3
W 03/21	L16 Perturbation Theory: Rayleigh-Schrödinger perturbation theory; Møller-Plesset perturbation theory; Multiconfigurational perturbation theory; MCSCF Methods; Parametrization of the MCSCF State
Week 10	
M 03/26	L17 Energy Derivatives and Molecular Properties: Geometrical derivatives; time-independent molecular properties; molecular gradients; molecular Hessians; response equations; uses of geometrical derivatives
W 03/28	L18 Coupled-Cluster Theory
Week 11	
M 04/02	L19 Discussion 4 Paper discussion on Coupled-Cluster Theory
W 04/04	Review session
Week 12	
M 04/09	**Exam II**
W 04/11	L19 DFT1 Foundations
Week 13	
M 04/16	L20 DFT2 Kohn-Sham equations; exchange correlation functionals
W 04/18	L21 Discussion 5 Discussion of papers on DFT
Week 14	
M 04/23	L22 Discussion 6
W 04/25	L23 Relativistic Quantum Chemistry
Week 15	
M 04/30	Code presentations
W 05/02	Code presentations
F 05/04	**Cookies and Refreshments**