Chem 571 Quantum Chemistry Fall 2014

Professor	**e-mail**	**Office Hour**	**Office**
Eitan Geva	eitan@umich.edu	Upon request	2000D Chem.

Prerequisites:

Chem 461/570 (or an equivalent introductory quantum mechanics course).

Website:

All course materials will be posted on the course CTools web site (https://ctools.umich.edu/).

Textbook:

Detailed lecture notes will be posted on the Course web site and can be used as a textbook.

The following book is also recommended as a reference: Quantum Mechanics, Volumes 1 & 2, C. Cohen-Tannoudji, B. Diu and F. Laloe (Willey).

Consulting other Quantum Mechanics texts that cover the same material on a similar level can be helpful.

Class Schedule:

Tuesday and Thursday 10:00 - 11:30 AM @ 1624 CHEM.

Grading:

6 Problem Sets 300 pts (50 per problem set).
Final exam 300 pts.

Total number of pts: 600 pts.

Problem sets and exam schedule:

	Submission deadline
Problem set #1	Sep 23
Problem set #2	Oct 7
Problem set #3	Oct 21
Problem set #4	Nov 11
Problem set #5	Nov 20
Problem set #6	Dec 4
Final Exam	Dec 9 (10:00-12:00AM)

Problem sets:

- Will be posted on the CTools web site no later than one week before submission deadline.
- Should be prepared legibly, with work shown in an orderly and logical manner. Numerical answers should be given in terms of correct units and highlighted.
- Should be submitted by the end of class on the designated day.

Tentative list of topics covered

1. General reminder: Classical mechanics, wave functions, stationary and time-dependent Schrodinger equations, stationary state, superposition principle.
2. Free particle wave packet dynamics.
3. Mathematical tools: Hilbert space, Dirac notation, Fourier transform, Dirac delta function, linear operators, Hermitian operators, unitary operators, representations in Hilbert space, eigenvalues and eigenvectors of operators, tensor product states and quantum correlations.
4. Postulates of Quantum Mechanics: postulates and their physical meaning, Heisenberg uncertainty principle, time evolution operator, Schrodinger, Heisenberg and interaction pictures, density operator.
5. The quantum harmonic oscillator: importance of vibrational dynamics, creation and annihilation operators, energy levels and stationary states, coherent state, canonical density operator.
6. Angular momentum: orbital angular momentum and its eigenvalues and eigenstates, rotational dynamics of molecules, general theory of quantum angular momentum, spin angular momentum, addition of angular momenta.
7. Electronic structure of atoms: particle in central field, Hydrogen atom, Hydrogen-like ions, multi-electron atoms, hybrid atomic orbitals.
8. Approximation methods: stationary and time dependent perturbation theory and the variational method.
9. Electronic structure of molecules: Born-Oppenheimer approximation, Hartree-Fock, Density Functional Theory and beyond.

Note: Departmental policy indicates the first step in inquiring about the accuracy of a final grade should be directed to the lead instructor of the course. This initial inquiry should take place within the first fifteen University business days of the first full term following the term in which the disputed grade was issued. If, after this inquiry, the student is not satisfied with the instructor's response, the student may choose to initiate a formal grade grievance. To initiate a formal grade grievance, the student should contact the Associate Chair of Undergraduate Studies (ACUS) of the home department of the course in question before the end of the fifth week of classes in the first full term following the term in which the disputed grade was issued.