Chemistry 7470 **Molecular Quantum Mechanics**
Fall 2006

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Recommended Texts:

Quantum Chemistry (5th edition) by Ira N. Levine
Elements of Quantum Mechanics, by Michael D. Fayer
Introduction to Quantum Mechanics by David J. Griffiths

Lectures: Mon, Wed, Fri 1:55 – 2:50 p.m. State Hall 113.

Grading:

Homework	40%
Mid-Term	25%
Final	35%

Homework: one assignment every two weeks (6 or 7 sets).

Note regarding homework: Due to the limitations of the single semester schedule, we will have very little time for solving problems in class. However, working through problems and examples is ***absolutely essential*** for mastering this subject. You will have to do a lot of independent studying in this course, both working through examples and assigned homework problems. I will be available for after-hours discussions on problem solving.

Course coverage:

The first part of this course will review at an accelerated pace the standard topics in quantum mechanics used in chemistry: quantum formalism, postulates, and notation; model systems such as particle in a box, rigid rotor, harmonic oscillator, and H atom; Variational Principle; Perturbation Theory; Spin and many-electron systems, Born-Oppenheimer approximation and electronic terms of diatomics, and principles of Hartree-Fock and Density Functional computational methods. The second part will consider more advanced topics including the quasiclassical (WKB) approximation, time-dependent perturbation theory and the foundations of spectroscopy, and the quantum dynamics in Liouville space (the density matrix).

CHM7470 Fall 2006 Tentative schedule of lecture topics

Date	Topics	Recommended reading*
Sept 6, 8, 11	The Wavefunction; The Schrödinger equation; Superposition Principle; Wavepackets; The Uncertainty principle.	Levine Ch. 1 Fayer Ch. 1, 3 Griffith Ch. 1, 2.1
Sept. 13, 15	Particle in a box; Tunneling; Particle in a 3D box: Degeneracy.	Levine Ch. 2 Fayer Ch. 5 Griffith Ch. 2.2, 2.5, 2.6
Sept. 18, 20, 22	Operators; Postulates of Quantum Mechanics; Schrodinger, Dirac, and matrix representation.	Levine Ch. 3, 7 Fayer Ch. 2, 4, 13 Griffith Ch. 3
Sept. 25, 27, 29	Harmonic oscillator and molecular vibrations. Raising and lowering operators.	Levine Ch. 4 Fayer Ch. 6 Griffith Ch. 2.3
Oct. 2, 4, 6	Angular Momentum in 2D (particle on a ring) and 3D (particle on a sphere or rigid rotor).	Levine Ch. 5 Griffith Ch. 4.3 Fayer Ch. 15
Oct. 9, 11	Hydrogen atom.	Levine Ch. 6 Fayer Ch. 7 Griffith Ch. 4.1, 4.2
Oct. 13	The Variation Principle. He atom.	Levine Ch. 8 Fayer Ch. 10 Griffith Ch. 7
Oct. 16, 18	Linear Variation Method. The Huckel model (tight-binding approximation). Band structure of solids.	Levine Ch. 8
Oct. 20, 23	Electron spin, Pauli exclusion principle. Bose-Einsten and Fermi-Dirac statistics. Slater determinants.	Levine Ch. 10 Griffith Ch. 4.4 Fayer Ch. 16
Oct. 25	*Midterm Exam*	
Oct. 27, 30, Nov. 1	Many-electron atoms. Addition of angular momenta. Terms symbols and Hund rules.	Levine Ch. 11 Fayer Ch. 15
Nov. 3, 6, 8	Diatomics: the Born-Oppenheimer approximation; electronic terms	Levine Ch. 13 Fayer Ch. 17
Nov. 10, 13	Introduction to ab initio methods: Hartree-Fock (mean field) approximation; Density functional.	Levine Ch. 11, 15
Nov. 15, 17	Quasiclassical approximation: WKB (Wentzel, Kramers, Brillouin)	Griffiths Ch. 8
Nov. 20, 22, Dec.1	Time-independent Perturbation Theory. Non-degenerate and degenerate cases. Secular equation.	Levine Ch. 9 Fayer Ch. 9 Griffith Ch. 6
Dec. 4, 6, 8	Time-dependent quantum mechanics. Time-dependent Perturbation Theory. Spectroscopy. Fermi Golden Rule.	Fayer Ch. 8, 11, 12 Levine Ch. 1, 9 Griffith Ch. 9
Dec. 11, 13, 15	Quantum Dynamics in Liouville space. The density matrix and quantum mechanics of statistical ensembles. Quantum Liouville equation.	Fayer Ch. 14
Dec. 18	Course Review	
Dec. 20	*Final Exam*	

* All lectures will be supplemented by handouts.