

Chemistry 521/421 Fall 2016

Atomic and Molecular Structure (Quantum Mechanics)

Instructor: Prof. Ed Castner

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Time: Mondays and Wednesdays, 08:40-10:00 (MORNINGS!) Location: WL-260

Text: *Elements of Quantum Mechanics*, by Michael D. Fayer

This syllabus offers a rough guide to what material will be covered, and when. Read the relevant chapters in the book *Elements of Quantum Mechanics* **before** the lectures. I urge you to download and print the lecture notes from the Sakai site before class, so that you can annotate the notes instead of transcribing each equation during lecture.

Homework problems for the relevant chapter should be done directly following lecture. Make sure to obtain and install Mathematica software to aid you in doing more complex problems. Any updates or changes to this schedule will be posted on Sakai. ***Instead of a final exam, there will be a take-home project due on Mon. 12/19/2015, 17:00.***

Course syllabus

Class 1	Wed., 9/7	Six postulates of QM; Chapter 1, <i>Elements, Mathematica</i>
Class 2	Tues. , 9/12	Chap. 2, <i>Elements</i> : wavefns., kets (bras), operators
Class 3	Wed., 9/14	Chap. 3, <i>Elements</i> : free particles, wavepackets
Class 4	Thurs., 9/19	Chap. 4, <i>Elements</i> : Dirac's Quantum Condition; Uncertainty
Class 5	Wed., 9/21	Chap. 5, <i>Elements</i> : Schrödinger equation
Class 6	Mon., 9/26	Chap. 5, <i>Elements</i> : particles in potentials- tunneling; ionization
Class 7	Wed., 9/28	Chap. 6, <i>Elements</i> : harmonic oscillator- Schrödinger rep.
Class 8	Mon., 10/3	Chap. 6, <i>Elements</i> : harm. osc.- Dirac- raising/lowering operators
Class 9	Wed., 10/5	Chap. 6, <i>Elements</i> : harm. osc. and time-resolved spectroscopy
Class 10	Mon., 10/10	Take home project due.
Class 11	Wed. 10/12	Chap. 7, <i>Elements</i> : H atom
Class 11	Mon., 10/17	Chap. 7, <i>Elements</i> : more on H atom
Class 12	Wed., 10/19	Chap. 8, <i>Elements</i> : time-dep. 2-state problems
Class 13	Mon., 10/24	Chap.9, <i>Elements</i> : perturbation theory. Non-degenerate, 1 st order
Class 14	Wed., 10/26	Chap.9, <i>Elements</i> : perturbation theory. 2 nd order, degenerate.
Class 15	Mon., 10/31	Chap. 10, <i>Elements</i> : He atom. perturbational, variational.
Class 16	Wed., 11/2	Chap. 11, <i>Elements</i> : time-dep. perturbation theory. Transitions.
Class 17	Mon., 11/7	Chap. 12, <i>Elements</i> : radiation: absorption, emission of photons.
Class 18	Wed., 11/9	Chap. 13, <i>Elements</i> : matrix representation
Class 19	Mon., 11/14	Chap. 13, <i>Elements</i> : more on the matrix representation
Class 20	Wed., 11/16	Chap. 14, <i>Elements</i> : density matrices- light/matter interactions
		Take home project due.
Class 21	Mon., 11/21	Chap. 14, <i>Elements</i> : more on density matrices.
no lecture	Wed., 11/23	no class- Friday class schedule
Class 22	Mon., 11/28	Chap. 15, <i>Elements</i> : angular momentum- raising/lowering ops.
Class 23	Wed., 11/30	Chap. 15, <i>Elements</i> : more on angular momentum
Class 24	Mon., 11/30	Chap. 16, <i>Elements</i> : electron spin
Class 25	Mon., 12/5	Chap. 16, <i>Elements</i> : more on electron spin
Class 26	Wed., 12/7	Chap. 17, <i>Elements</i> : covalent bonds- H ₂ ⁺ and H ₂
Class 27	Mon., 12/12	Chap. 17, <i>Elements</i> : more on covalent bonds
Class 28	Wed. 12/14	Chap. 17, <i>Elements</i> : chemical bonding