Course Syllabus: CH651 Molecular Quantum Mechanics I

Fall 2014, Prof. D.F. Coker

Recommended Texts:

(1) Quantum Mechanics in Chemistry (George C. Schatz and Mark A. Ratner)
(2) Chemical Dynamics in Condensed Phases (Abraham Nitzan)

Evaluation: Assignments: 30%, Midterm: 30%, Final: 40%

Office Hours: SCI530 Monday afternoon after 1pm

Review of Classical Mechanics

- Classical equations of motion
- Phase space, the classical distribution function and the Liouville equation

Review of Quantum Mechanics

- The wave function and the time dependent Schrodinger Equation
- Statistical Interpretation – Normalization, Expectation Values, Operators
- Stationary States, Hermiticity, Hilbert Spaces
- Simple One Dimensional Models

Quantum Dynamics Using the Time Dependent Schrodinger Equation

- Formal Solutions
- The two level system in a time dependent field
- Nuclear potential surfaces
- Representations: Schrodinger, Heisenburg, Interaction
- Time-dependent perturbation theory
- Quantum dynamics of free particles
- Quantum dynamics of harmonic oscillators
- Tunneling

Interaction of Radiation with Matter

- Electromagnetic fields
- Interaction between matter and field

- Absorption and emission of light
- Light scattering

Occupation number representations

- Harmonic molecular vibrations and quantized radiation fields
- Occupation number representations for electrons
- Fermion field operators and second quantization
- Molecular electronic structure: Model hamiltonians and occupation number representations

Time correlation functions

- Diffusion, Golden rule rates, optical absorption
- Classical and quantum time correlation functions
- Harmonic baths and the spin boson model

Electron transfer processes

- A primitive model
- Continuum dielectric theory
- Molecular theory of nonadiabatic electron transfer
- Solvent-controlled electron transfer dynamics
- Reorganization energy and the Marcus parabolas

Spectroscopy

- Molecular spectroscopy
- Raman scattering
- Thermal relaxation and dephasing
- Optical response functions