**Department of Chemistry Syllabus**

This syllabi is advisory only. For details on a particular instructor's syllabus (including books), consult the instructor's course page. For a list of what courses are being taught each quarter, refer to the Courses page. *Every instructor has prerogative to teach the course as they see fit and ultimately the instructor's syllabus supersedes all others.*

***CHE 210B: Time-Dependent Quantum Mechanics in Physical Chemistry***

Approved:

Suggested Textbook: (actual textbook varies by instructor; check your instructor)

TBA

Suggested Schedule:

I. INTRODUCTION

Time-dependent Schrödinger equation

II. WAVE PACKETS

Dynamics of wave packets

Continuity equation

Quantum flux. Bohmian trajectories, Bohmian interpretation of QM

Sudden jump approximation. "Shake up" (Migdal) transitions

III. HARMONIC OSCILLATOR

Coherent States

Wigner function

Short and long laser pulses

Dynamics of vibrational wave packets and Femtochemistry.

IV. EVOLUTION OPERATOR

Representations

Heisenberg picture

V. DYNAMICS OF MULTILEVEL QUANTUM SYSTEM

Mixing of quantum states

General solution

VI. TWO-LEVEL SYSTEM AND ITS APPLICATIONS

Resonant and non-resonant two-level systems

Dynamics of two-level systems

Tunneling dynamics

Double-well problem. Proton tunneling

Quasiclassical transmission coefficient

VII. THREE-LEVEL SYSTEM

Virtual transitions. Coupling through a bridge. Superexchange

Green functions

Electron tunneling in proteins

Principles of STM

VII. MULTILEVEL QUANTUM SYSTEMS

Dephasing and rephasing

Quantum beats. Intramolecular Vibrational Relaxation (IVR).

Intensity of "forbidden" transitions. Overtone transitions

VIII. QUANTUM RELAXATION

Irreversibility

Golden Rule

IX. COLLISION THEORY

Time-dependent and time-independent pictures

Born formula

Elastic and inelastic collisions

X. TIME-DEPENDENT PERTURBATION

Interaction representation.

Perturbation theory results

XI. INTERACTION OF RADIATION WITH MATTER

Dipole, quadrupole, multipole transitions

Transition matrix elements

XII. QUANTUM RADIATION

Quantization of radiation

Photons, coherent states, and classical coherent radiation

XIII. RADIATIVE DECAY

Life-time of excited states

XIV. PERIODIC TIME-DEPENDENT PERTURBATION

Dressed states

Strong fields. Coherent excitation. Rabi oscillations

Weak field. Incoherent absorption. Absorption cross section

XV. MULTIPHOTON PROCESSES

Short laser pulses and radiation of high intensity

Multiphoton absorption

Rayleigh and Raman scattering

Coherent anti-Stokes Raman Spectroscopy and IVR

Nonlinear optics

XVI. ELECTRONS AND NUCLEI IN MOLECULES

Born-Oppenheimer approximation

Non-adiabatic transitions. Landau-Zener theory

Conical intersection. Berry phase

Vibrational dynamics/mixing in polyatomic molecules. IVR

Vibrational superxchange. Dynamic tunneling

Relaxation in liquids and biological systems.

Pump-Probe experiments. Time-resolved Stokes shift spectroscopy

XVII. ELECTRONS AND PHONONS IN SOLIDS

Electron-phonon interaction

Superconductivity and three-level system

Josephson contact and the two-level system

XVIII. THEORY OF RATES OF CHEMICAL REACTIONS

Transition state theory

Tunneling. Proton transfer reactions

RRKM

Electron transfer theory

XIX. QUANTUM MECHANICS AND STATISTICS

Density matrix

Quantum decoherence. EPR paradox

NMR. Bloch equations

Motional narrowing

XX. CORRELATION FUNCTIONS

Linear response theory

Kubo formalism

Rates and transport coefficients

Additional Notes:

Prerequisite: course 210A

Learning Goals:

Matrix mechanics and time-dependent quantum chemistry: matrix formulation of quantum mechanics, Heisenberg representation, time-dependent perturbation theory, selection rules, density matrices, and miscellaneous molecular properties