CHEM 825: Quantum Dynamics with Applications to Spectroscopy

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Course Outline:

I. Review of Basic Wavemechanics Results: Useful Basis Sets

- A. Particle-in-a-Box
- B. Harmonic Oscillator
- C. Hydrogen Atom

II. Introduction to Quantum Algebra

- A. Harmonic Oscillator
- B. Angular Momentum

III. Matrix Formulation of Quantum Mechanics

- A. Representation of States and Operators
- B. Eigenstates by Matrix Diagonalization
- C. Change of Basis Relations

IV. The Dynamics of Spectroscopic Transitions

- A. Rabi Solution and Feynman-Vernon-Hellwarth Approach
- B. First-Order Time-Dependent Perturbation Theory: Fermi's Golden Rule
- C. Time-Independent Solution through Dressed States: Autler-Townes Effect

V. Methods for Ensembles

- A. The Density Matrix and Coherence
- B. Phenomenological Treatment of Relaxation: T_1 and T_2
- C. Pulse Sequences for NMR Spectroscopy
- D. Motional Effects in the Spectrum (Anderson and Kubo Theory)

VI. Radiationless Processes: Dynamics of Excited States

- A. Dynamics in Excited Electronic States (Rydberg Atoms)
- B. Intramolecular Vibrational Dynamics
- C. Dynamics in Condensed Phases (Matrices, Solutions, and Surfaces)