

Chemistry 881 Lecture Topics Fall 2001

Texts

PHYSICAL CHEMISTRY A Molecular Approach

McQuarrie and Simon

MATHEMATICS for PHYSICAL CHEMISTRY, Mortimer

i. Mathematics Review (M, Chapters 1,2,3 & 4; M&S, Chapters A & C)

Trigonometric Functions

Elementary functions

Series representations

Complex numbers

Derivatives of a single variable

One dimensional Integrals

Derivatives of functions with several variables

ii. Introduction to Mathematica

A. Historically Significant Experiments (M&S,Chapter 1)

Blackbody Radiation

Photoelectric effect

Compton effect

DeBroglie Wavelength

Atomic spectra are not continuous (line spectra)

Heisenberg Uncertainty Principle

B. The Classical Wave Equation (M&S, Chapter 2)

The Wave Equation and its properties

Separation of variables

General solution

Normal modes

Linear differential equations with constant coefficients

Two dimensional Wave Equation

C. Particle on a line/in a box (M&S, Chapter 3)

Model

Classical expectations

Time dependent Schrodinger equation

Time independent Schrodinger equation

Wavefunction

Eigenvalue equation

Hamiltonian operator

Linear operator

Solution to time independent Schrodinger equation

Boundary conditions

Stationary states

Energy levels

Quantum number

Wavefunctions

Orthogonality

Normalization

Probability interpretation
Correspondence principle
Expectation values
Uncertainty principle
General time dependent solution

ii. Math Review (M, Section 5.7)

Multiple Integrals

D. Particle in a plane/particle in a two dimensional box (not in text)

Time independent Schrodinger equation
Boundary conditions
Separability
Energy levels
Degeneracy
Wavefunctions
Orthogonality
Symmetry
Probability interpretation
General time dependent solution

E. Particle in a cube (M&S, Chapter 3)

Time independent Schrodinger equation
Boundary conditions
Separability
Energy levels

Degeneracy

Wavefunctions

Orthogonality

Symmetry

Probability interpretation

General time dependent solution

F. Harmonic oscillator (M&S, Chapter 5)

Model

Classical expectations

Time dependent Schrodinger equation

Time independent Schrodinger equation

Eigenvalue equation

Hamiltonian operator

Linear operator

Solution to time independent Schrodinger equation

Boundary conditions

Stationary states

Energy levels

Quantum number

Wavefunctions

Orthogonality

Normalization

Probability interpretation

Correspondence principle

Expectation values

Uncertainty principle

General time dependent solution

Diatomic molecules and vibrational spectroscopy

G. Postulates & Principles of Quantum Mechanics (M&S, Chapter 4)

Postulate 1

Postulate 2

Postulate 3

Postulate 4

Postulate 5

Commuting operators

H. Rigid Rotor (M&S, Chapter 5)

Classical motion

Spherical coordinates

Moment of inertia

Angular momentum

Schrodinger equation

Separation of variables

Wavefunctions

Spherical harmonics

Energy levels

Linear molecules

Rotational spectroscopy

I. Hydrogen atom (M&S, Chapter 6)

Model

Time independent Schrodinger equation

Separation of variables

Energy levels

Degeneracy

Wavefunctions

Radial functions

Angular functions

s,p,d,f,g,...functions

Probability density

Radial distribution function

Contour surfaces

iii. Mathematics review (M&S, Chapter E)

Determinants

J. Approximation methods (Chapter 7)

Variation method

Trial function

Boundary conditions

Linear variation function

Secular determinant

Perturbation theory

K. Multielectron atoms (M&S, Chapter 8)

Atomic units

Hamiltonian Operator

Variational calculations on He atom

Electron spin

Hartree-Fock equations

Correlation energy

Antisymmetry principle

Slater determinants

Term symbols

Coupling of angular momenta

Equivalent versus non-equivalent electrons

Hund's rules

L. Chemical bond & diatomic molecules (M&S, Chapter 9)

Born-Oppenheimer approximation

Schrodinger hamiltonian

Linear combination of atomic orbitals for H_2^+

Binding energy of H_2^+

Electronic configuration of first row diatomics

Photoelectron spectra

Heteronuclear diatomics

M. Bonding in polyatomic molecules (M&S, Chapter 10)

sp, sp², sp³, Hybrid orbitals

Photoelectron spectra

Huckel theory

N. Computational Quantum Chemistry (M&S, Chapter 11)

Basis sets

Hartree-Fock wavefunctions

The Gaussian program

The Spartan program

Role of Computational Chemistry

O. Molecular spectroscopy (M&S, Chapter 13)

Electromagnetic spectrum & molecular processes

Diatomic molecules

Rotation-vibration spectroscopy

Rotational spectroscopy

Anharmonicity in vibrational spectroscopy

Excited electronic states

Electronic spectra