

## **I. Classical Mechanics and Particle Nature of Light**

- (1) Short history of physics
- (2) Energy of a particle (classical view)
- (3) Electromagnetic wave (classical view)
- (4) Photoelectric effect
- (5) Hydrogen atom emission spectrum
- (6) Dual nature of light

## **II. Wave Nature of Matter**

- (1) The de Broglie hypothesis
- (2) Hydrogen atom (model)
- (3) Interaction of light and matter
- (4) The Heisenberg uncertainty principle

## **III. The Schrodinger Equation**

- (1) A brief history of quantum mechanics
- (2) 1-dimensional (1D) Schrodinger equation
- (3) Physical meaning of wavefunction
- (4) 1-dimensional (1D) particle in a box (PIB)
- (5) Harmonic oscillator (classical) : Review
- (6) Vibration of diatomic molecule: 1D quantum harmonic oscillator
- (7) Complete solutions of quantum harmonic oscillator
- (8) Infra-red (IR) spectrum of diatomic molecule

## **IV. Mathematical Machinery of Quantum Mechanics**

- (1) Wavefunction (postulate #1)
- (2) Quantum mechanical operator (postulate #2)

- (3) Eigenvalue equation (postulate #3)
- (4) Free particle
- (4) Expectation (average) value of physical property (postulate #4)
- (5) Orthogonality of eigenfunctions
- (6) Commutator

## **V. Quantum Mechanics in Multi-Dimensions**

- (1) The 3-dimensional (3D) Schrodinger equation
- (2) 3-dimensional (3D) particle in a box (PIB)
- (3) Classical mechanics of rotation
- (4) Quantum mechanics of 3-dimensional rotation
- (5) Rotational wavefunctions
- (6) Microwave spectroscopy
- (7) Angular momentum in quantum mechanics

## **VI. Hydrogen Atom**

- (1) Hydrogen atom in spherical polar coordinates
- (2) Schrodinger equation (electronic)
- (3) Angular part of the solution
- (4) Radial part of the solution
- (5) Radial probability distribution
- (6) Atomic orbitals of hydrogen atom
- (7) Electron spin

## **VII. Multi-Electron Atoms**

- (1) The variational method
- (2) Helium atom

- (3) Hartree-Fock (HF) self-consistent field (SCF) method
- (4) Electron spin in multi-electron wavefunctions
- (5) Schrodinger equation for many-electron atoms

### **VIII. Molecular Quantum Mechanics**

- (1) Hydrogen molecular ion:  $H_2^+$
- (2) Born-Oppenheimer approximation
- (3) Procedure to solve molecular Schrodinger equation
- (4) Electronic transition: UV-Vis absorption
- (5) Solving electronic Schrodinger equation: LCAO method
- (6) LCAO and Aufbau principle for molecule