### Know, understand, and be able to use key equations:

- 1. Time-dependent Schrödinger equation.
- 2. Time-independent Schrödinger equation
- 3. Fermi's golden rule
- 4. Time-correlation formulation for spectral broadening

## **Understand key concepts/notation:**

- 1. Bra-ket notation.
- 2. Hermitian operators
- 3. eigenfunctions/eigenvalues
- 4. expansion in a complete orthonormal set
- 5. Dirac delta function
- 6. Commutators/Simulataneously observable operators
- 7. Heisenberg Uncertainty Principle
- 8. De Broglie wavelength
- 9. Planck's law
- 10. Expectation values
- 11. Probabilistic interpretation of the wavefunction
- 12. Slater determinants
- 13. Allowable and non-allowable wavefunctions.
- 14. Allowable and non-allowable operators.

# Ground-state wavefunctions, eigenenergies, quantum numbers, and selection rules for:

- 1. Particle-in-a-box.
- 2. Harmonic Oscillator
- 3. Rigid Rotor
- 4. One-electron atom
- 5. Angular momentum (L, S, J, etc.)

### **Atoms & Molecules:**

- 1. Concept of effective nuclear charge.
- 2. Hartree-Fock
- 3. Molecular orbital theory; linear combination of atomic orbitals
- 4. Valence bond theory.
- 5. Term Symbols
- 6. Hund's Rules
- 7. Born-Oppenheimer Approximation

### Computational methods/approaches.

- 1. Perturbation Theory
- 2. Variational Principle
- 3. Evaluating expectation values
- 4. "Fundamental experiments" of quantum mechanics like blackbody radiation and the photoelectric effect.
- 5. Hartree-Fock