Chapter 9 - 2, 3, 4, 5, 6, 7, 13, 16, 23a

Chapter 8 - Suggested Chapter problems
1-7, 9, 10a-d, 12, 13, 14, 16, 18, 19, 21a, 22, 25

Chapter 9 Reading - Skip "Tunneling" pp. 463-464
DO Read "Harmonic Osc" pp. 464-5 - 467
Skip "Rigid Rotator" pp. 468-469
DO Read "Hydrogen Atom" and sections following
ie pp. 469 - 470
Skip "Many Electron Atoms" pp. 476 - 478
Read lightly 479-490. Skip 491-513

Review past 2 lectures - Chapter 9

Wave-particle duality - small particles show wave-like props

Describe wave behavior by wave function: \( \psi(x, y, z) \)

\[ \psi^2(x, y, z) \rightarrow \psi^2 \propto \text{Probability of finding } \psi \text{ at } x, y, z \]

Finite Probability:

\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi^2 dx dy dz = 1
\]

Operator \( \equiv \) Expectation Value

\[
\overline{\psi} = \int \psi^* \psi N \, dV
\]

\[
E = \int \psi^* \mathcal{H} \psi N \, dV
\]

\[
\mathcal{H} = \frac{-\hbar^2}{2m} \Delta + V(x)
\]

One Dimension
One Dimensional
Particle in a Box – A really simple atom

Use \( \int_{-\infty}^{\infty} N^2 dx = 1 \) and Boundary Conditions to yield

\[
\psi_n = \sqrt{\frac{2}{a}} \sin \left( \frac{n\pi}{a} x \right)
\]

\[
E_n = \frac{\hbar n^2}{8ma^2}
\]

\[
\lambda = \frac{8ma^2}{\hbar (2n+1)}
\]

\( N = \text{quantum number of the highest filled orbital} \)
(For simple atom, \( N = \frac{1}{2} (\pm \text{electrons}) \))

Particle in a Box had a very simple \( U(x) \).

Fancier Version

F = -kx

\( U = \frac{1}{2} kx^2 \)

\( \psi = \cos \) or \( \sin \)

Harmonic Oscillator

\[ H = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \]

\( x = \text{deviation from lowest } E \text{ length} \)

Elaborate why
Again, one-dimensional

\[ \frac{d^2 \psi}{dx^2} + \frac{1}{2} k x^2 \psi = E \psi \]

\( \psi \)

Bonding Orbital

Note similarities

\[ U(x) \]

\( x \rightarrow \)

Good descriptor for \textit{Bond} wavefunctions

Quantized energy levels \( \Rightarrow n = 1, 2, 3, 4, \ldots \)

Harmonic oscillator is used as a wavefunction

for many \( \text{a molecular dynamics and molecular mechanics} \)

\( \text{Calculations. NOT BAD} \)
H Atom - 3 Dimensions / move from \( x, y, z \) to polar coords.

\[ H = \frac{-e^2}{4\pi\varepsilon_0 r} \]

radius of \( e^0 \) from center (nucleus)

3 QUANTUM NUMBERS - POLAR COORDS

\( n, l, m \)

radial  angular  

\( E_n = -\frac{\mu e^4}{2\hbar^2 n^2} \)

Back to General Chemistry

quantized values for energy

\( n = 1, 2, 3, \ldots \)

READ pp 469-476
H-atom

Read lightly pp 479-490 and relate it back to your General and Organic Chemistry

Skip 491-513. Read 514-517

Heisenberg Uncertainty Principle

\[ \Delta p \Delta x \geq \frac{1}{2} \left( \frac{\hbar}{2\pi} \right) = \frac{1}{2} \hbar \]

\( \frac{m\nu}{\lambda} \) relates to 

\( \nu \rightarrow \text{Position} \)

\( \lambda = \frac{\hbar}{m\nu} \)

CANNOT KNOW BOTH

WAVE  PARTICLE

TO HIGH ACCURACY