# 1 Chapter 1

- Energy E of a photon of light in eV:

$$\lambda = \frac{1.24eV}{E}$$

- Distance D between adjacent planes in cubic lattices:

$$D = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

- Angle between 2 Miller index directions A and B:

$$\cos\theta = \frac{A \bullet B}{|A||B|}$$

# 2 Chapter 2

- Planck relationship:

$$E = hv = (\frac{h}{2\pi})(2\pi v) = \hbar\omega$$

- Classical energy of a particle:

$$\frac{1}{2}mv^2 = \frac{1}{2}\frac{m^2v^2}{m} = \frac{\rho^2}{2m}$$

- De Broglie:

$$\lambda = \frac{h}{\rho} = \frac{h}{mv} \Rightarrow \rho = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k$$

- Momentum or energy in terms of k can be derived by combining De Broglie with the classical energy of a particle:

$$E = \hbar\omega = \frac{\rho^2}{2m} = \frac{\hbar^2k^2}{2m}$$

- Rydberg Constant:

$$R = 109,678cm^{-1}$$

- Lyman:

$$v = cR(\frac{1}{1^2} - \frac{1}{n^2}), n = 2, 3, 4, ...$$

- Balmer:

$$v = cR(\frac{1}{2^2} - \frac{1}{n^2}), n = 3, 4, 5...$$

- Paschen:

$$v = cR(\frac{1}{3^2} - \frac{1}{n^2}), n = 4, 5, 6, ...$$

- Postulate for Bohr:

$$\rho_0 = n\hbar, n = 1, 2, 3, 4, ...$$

- Finding radial forces on orbiting electron:
  (Electrical force toward nucleus) = (Equivalent force in terms of radial acceleration)

$$-\frac{q^2}{kr^2} = -\frac{mv^2}{r}$$

$$\rho_0 = n\hbar = mvr \Rightarrow mv^2 = \frac{m^2v^2}{m} = \frac{n^2\hbar^2}{mr^2}$$

$$\frac{q^2}{kr^2} = \frac{1}{mr}\frac{n^2\hbar^2}{r^2} \Rightarrow r_n = \frac{kn^2\hbar^2}{mq^2}$$

  $|r_n$ is the radius of the nth orbit

$$-\frac{q^2}{kr^2} = -\frac{mv^2}{r} \Rightarrow \frac{n\hbar}{rm} = \frac{q^2}{kn\hbar}$$

  by subbing r from above.

  $\Rightarrow$ K.E. of $e^- =$

$$\frac{1}{2}mv^2 = \frac{mq^4}{2k^2n^2\hbar^2}$$

  P.E. of $e^- =$

$$-\frac{q^2}{kr_n} = -\frac{mq^4}{k^2n^2\hbar^2}$$

  by subbing r

  Total Energy of $e^- =$

$$E_n = KE = PE = -\frac{mq^4}{2k^2n^2\hbar^2} = -KE$$

- Energy difference between orbits:

$$E_{n2} - E_{n1} = \frac{mq^4}{2k^2\hbar^2}(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

- Frequency of light given by a transition between orbits:

$$V_{21} = \left[\frac{mq^4}{2k^2\hbar^2 h}\right](\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

- Heisenberg uncertainty principle:
  $(\Delta x)(\Delta \rho_x) \geq \frac{\hbar}{2}$
  $(\Delta E)(\Delta t) \geq \frac{\hbar}{2}$

## 2.1 Quantum Mechanics

| Classical Variable | $\rightarrow$ | Quantum Operator |
|---|---|---|
| $x$ | $\rightarrow$ | $x$ |
| $f(x)$ | $\rightarrow$ | $f(x)$ |
| $\rho(x)$ | $\rightarrow$ | $\frac{\hbar}{j}\frac{\partial}{\partial x}$ |
| E | $\rightarrow$ | $-\frac{\hbar}{j}\frac{\partial}{\partial t}$ |

- Normalization of the probability density (the wave function is the probability density):
$$\int_{-\infty}^{\infty} \Psi^* \Psi dxdydz = 1 \tag{1}$$

- Time averaged expectation of the particle state
$$< Q >= \int_{-\infty}^{\infty} \Psi^* Q_{op} \Psi dxdydz \tag{2}$$

- Classical energy of a partical:
$$KE + PE = E \Rightarrow \frac{1}{2}mv^2 + V = E$$
$$\frac{1}{2}mv^2 = \frac{1}{2}\frac{(mv)^2}{m} = \frac{1}{2}\frac{\rho^2}{m} = \frac{\rho^2}{2m} \Rightarrow \frac{\rho^2}{2m} + V = E \tag{4}$$
$$\rho \rightarrow \frac{\hbar}{j}\frac{\partial}{\partial x}, E \rightarrow -\frac{\hbar}{j}\frac{\partial}{\partial t}$$
$$\Rightarrow \frac{-1}{2m}\hbar\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) = \frac{-\hbar}{j}\frac{\partial \Psi(x,t)}{\partial t}$$

  where
$$(\frac{\partial}{\partial x})^2 \rightarrow \frac{\partial^2}{\partial x^2}, j^2 = -1$$

- Wave function in 3D then:
$$\frac{-\hbar}{2m}\nabla^2\Psi + V\Psi = \frac{-\hbar}{j}\frac{\partial \Psi}{\partial t} \ni \nabla^2\Psi = \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \tag{5}$$

- Separation of variables:
$$\frac{-\hbar}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = \frac{-\hbar}{j}\frac{\partial \Psi(x,t)}{\partial t} \tag{6}$$

$$\Rightarrow$$

$$-\frac{\hbar}{2m}\frac{\partial^2\psi(x)}{\partial x^2}\phi(t)+V(x)\psi(x)\phi(t)=-\frac{\hbar}{j}\psi(x)\frac{\partial\phi}{\partial t} \tag{7}$$

$$\Rightarrow$$

$$\frac{d\phi(t)}{dt}+\frac{j}{\hbar}E\phi(t)=0 \tag{8}$$

(time dependent portion)

$$-\frac{\hbar}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x) \tag{9}$$

(time independent portion)

- E $\equiv$ equivalent constant, corresponds to total energy of the particle
- Wave function as linear combination of various eigenfunctions

$$\psi(x,t)=_n C_n\Psi_n e^{-j\frac{E_n}{\hbar t}} \ni E_n \equiv nth\ prefactor \tag{10}$$

- Infinite potential well

$$V(x)=\begin{cases} 0 & ,x\neq 0andx\neq L \\ \infty & ,x=0orx=L \end{cases}$$

$$\Rightarrow$$

$$(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x))\psi(x)=E\psi(x)\Rightarrow\frac{d^2\psi(x)}{dx^2}=\frac{2m}{\hbar}E\psi(x) \tag{11}$$

$$\Rightarrow$$

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}E\psi(x)=0 \tag{12}$$

$$\Rightarrow$$

$$\psi(x)=\{\sin(kx),\cos(kx)\}\ni k=\frac{\sqrt{2mE}}{\hbar} \tag{13}$$

$$\cos(kx)0whenx=0\Rightarrow A\sin(kx)isoursolution.\ni k=\frac{\sqrt{2mE}}{\hbar} \tag{14}$$

$$whenpotentialis0atx=0andL,k=\frac{n\pi}{L},n=\{1,2,3,...\} \tag{15}$$

$$therefore:\frac{\sqrt{2mE_n}}{\hbar}=\frac{n\pi}{L}\Rightarrow E_n=\frac{n^2\pi^2\hbar^2}{wmL^2} \tag{16}$$

- A is found by normalizing the probability densiyt integral

$$\int_{-\infty}^{\infty} \Psi^* \Psi dx = \int_0^L A^2 \sin^2(\frac{n\pi x}{L})dx = A^2 \frac{L}{2} review\ trig\ calc\ and\ show\ the\ process\ here \tag{17}$$

Set the above to 1 to find A

$$\frac{A^2 L}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{L}} \tag{18}$$

$$Therefore:\ \psi = \sqrt{\frac{2}{L}} \sin(\frac{n\pi}{L})\ for\ an\ infinite\ well \tag{19}$$

- Parabolic Potential Well (simple harmonic oscillator)

$$V(x) = kx^2, E_n = (n + \frac{1}{2})\hbar\omega \tag{20}$$

- Coulombic Potential Well

$$\frac{d^2}{d\phi^2}\Phi + m^2\Phi = 0 \Rightarrow \Phi_m(\phi) = Ae^{jm\phi} \tag{21}$$

$$1 = \int_0^{2\pi} \Psi^* \Psi d\psi \Rightarrow \int_0^{2\pi} \Phi_m^*(\phi)\Phi_m(\phi)d\phi = 1 \tag{22}$$

$$\Rightarrow A^2 \int_0^{2\pi} e^{-jm\phi} e^{jm\phi} d\phi \tag{23}$$

$$\Rightarrow$$

$$A^2 \int_0^{2\pi} d\phi = 2^2 \tag{24}$$

$$\Rightarrow$$

$$A = \frac{1}{\sqrt{2\pi}} \Rightarrow \Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{jm\phi} \tag{25}$$

$$\ni m = \{..., -3, -2, -1, 0, 1, ...\}$$

similar for $\Theta_l(\theta) and R_n(r) Atomic numbers describing allowable states in a hydrogen atom$
n = 1,2,3,...
l=0,1,2,3,...,n-1
m (m$_l$) = $-l, ..., -2, -1, 0, 1, 2, ..., l$
$s(m_s) = \frac{\pm\hbar}{2}$

- | n | l | m | $\frac{s}{\hbar}$ | Allowable states in subshell | Allowable states in complete shell |
  |---|---|---|---|---|---|
  | 1 | 0 | 0 | $\pm\frac{1}{2}$ | 2 | 2 |
  | 2 | 0 | 0 | $\pm\frac{1}{2}$ | 2 | |
  | 2 | 1 | -1 | $\pm\frac{1}{2}$ | | 8 |
  | 2 | 1 | 0 | $\pm\frac{1}{2}$ | 6 | |
  | 2 | 1 | 1 | $\pm\frac{1}{2}$ | | |
  | 3 | 0 | 0 | $\pm\frac{1}{2}$ | 2 | 18 |
  | 3 | 1 | -1 | $\pm\frac{1}{2}$ | | |
  | 3 | 1 | 0 | $\pm\frac{1}{2}$ | 6 | 18 |
  | 3 | 1 | 1 | $\pm\frac{1}{2}$ | | |
  | 3 | 2 | -2 | $\pm\frac{1}{2}$ | | |
  | 3 | 2 | -1 | $\pm\frac{1}{2}$ | | |
  | 3 | 2 | 0 | $\pm\frac{1}{2}$ | 10 | 18 |
  | 3 | 2 | 1 | $\pm\frac{1}{2}$ | | |
  | 3 | 2 | 2 | $\pm\frac{1}{2}$ | | |

- n is the principle atomic number
- l is the number that determines s,p,d,f,g,...

# 3 Chapter 3

- Equilibrium number of EHP's in pure Si at room temp:

$$10^{10}\frac{EHP}{cm^3}$$

- Si atom density in pure Si at room temp:

$$5 * 10^{22}\frac{atoms}{cm^3}$$