# Formula Sheet

# **Physical Constants:**

Quantity	Symbol, equation	Value
Speed of light	C	$2.9979 \times 10^8 \text{ m s}^{-1}$
Electron charge	e	$1.602 \times 10^{-19}$ C
Planck constant	h	$6.626 \times 10^{-34} \text{Js}$
Planck constant, reduced	$\hbar = h/2\pi$	$1.055 \times 10^{-34} \text{ J s}$
Conversion constant	$\hbar c$	197.327 MeVfm = 197.327 eVnm
Electron mass	$m_e$	$9.109 \times 10^{-31} \text{ kg} = 0.511 \text{MeV/c}^2$
Proton mass	$m_p$	$1.673 \times 10^{-27} \text{ kg}^2 = 938.272 \text{MeV/c}^2$
Neutron mass	$m_n$	$1.675 \times 10^{-27} \text{ kg} = 939.566 \text{MeV/c}^2$
Fine structure constant	$\alpha = e^2/\hbar c$	1/137.036
Classical electron radius	$r_e = e^2/m_e c^2$	$2.818 \times 10^{-15} \text{ m}$
Electron Compton wavelength	$\lambda = h/m_e c = r_e/\alpha$	$2.426 \times 10^{-12} \text{ m}$
Proton Compton wavelength	$\lambda = h/m_p c$	$1.321 \times 10^{-15} \text{ m}$
Bohr radius	$a_0 = r_e/\alpha^2$	$0.529 \times 10^{-10} \text{ m}$
Rydberg energy	$\mathcal{R} = m_e c^2 \alpha^2 / 2$	$13.606 \mathrm{eV}^{-11} \mathrm{MeVT}^{-1}$
Bohr magneton	$\mu_B = e\hbar/2m_e$	$5.788 \times 10^{-11}$
Nuclear magneton	$\mu_N = e\hbar/2m_p$	$3.152 \times 10^{-14} \mathrm{MeVT^{-1}}$
Avogadro number	$N_A$	$6.022 \times 10^{23} \text{ mol}^{-1}$
Boltzmann constant	k	$1.381 \times 10^{-23} \text{ J K}^{-1}$
		$= 8.617 \times 10^{-5} \text{eVK}^{-1}$
Gas constant	$R = N_A k$	$8.31 \text{ J mol}^{-1} \text{ K}^{-1}$
Gravitational constant	G	$6.673 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$
Permittivity of free space	$\epsilon_0 = 1/\mu_0 c^2$	$8.854 \times 10^{-12} \text{Fm}^{-1}$
Permeability of free space	$\mu_0$	$4\pi \times 10^{-7} \text{ N A}^{-2}$

### Conversion of units:

 $1 \text{fm} = 10^{-15} \text{ m}, 1 \text{fm} = 10^{-15} \text{ m}, \quad 1 \text{ barn} = 10^{-28} \text{ m}^2 = 100 \text{fm}^2, 1 \text{ atmosphere} = 101325 \text{ Pa}, \quad \text{Thermal energy at } T = 300 \text{ K}: \quad kT = [38.682]^{-1} \text{eV} \ 0^{\circ}\text{C} = 273.15 \text{ K}, \quad 1 \text{eV} = 1.602 \times 10^{-19} \text{ J}, \quad 1 \text{eV/c}^2 = 1.783 \times 10^{-36} \text{ kg}$ 

#### Properties of the Solution of 1D stationary Schrodinger Equation:

- 1. For 1D potential, all stationary solutions are non-degenerate.
- 2. Stationary square integrable solution exist only for E > minV(x)
- 3. If V(x) is real, then  $\Psi(x)$  can be taken to be real.
- 4. Eigenvalues of a Hermitian Hamiltonian are all real.
- 5. The eigenfunctions of a Hermitian operator form a complete orthogonal basis set, for smooth potentials.
- 6. 1D Schrödinger equation Solution is real up to an over all phase.
- 7. For a given 1D even potential the stationary states are either even or odd.
- 8. The wave function and its first order space derivative is continuous all over space and in particular at the boundaries of a finite potential.
- 9. At boundaries with Dirac delta function potential, the first space derivative of the wavefunction is discontinuous.
- 10. Physical solution should be finite all over space, no blow ups, in particular at infinity.
- 11. The number of nodes (zeros) of the eigenfunction increases by one unit as we move from the ground state (zero nodes) to higher excited states.
- 12. Bound states exist only for confining potential (classically between turning points of the potential).

### The Origin of Quantum Physics:

$$E = h\omega p = \frac{h}{\lambda} = \hbar k (1)$$

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$$\lambda = \frac{h}{p} \lambda_C = \frac{h}{mc} (2)$$

# Blackbody Radiation:

Plank energy spectral density: 
$$\rho(\nu) = \frac{8\pi h \nu^3}{c^3} \left[ \frac{1}{\exp\left(\frac{h\nu}{k_B T}\right) - 1} \right]$$

#### Photoelectric Effect:

W is the work function of irradiated metal.  $V_s$  is the stopping potential.

$$K = \frac{1}{2} mv^2 = h\nu - W = \frac{hc}{\lambda} - W \; ; \quad K = \frac{1}{2} mv^2 = |e|V_s \leftrightarrow V_s = \frac{K}{|e|}$$

$$\nu \ge \frac{W}{h} = \nu_{\min}; \quad \nu = \frac{1}{T} = \frac{c}{\lambda}; \quad \nu = \frac{\omega}{2\pi}$$

#### de Broglie Formula:

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

### Bohr Hydrogen-like Atom:

$$E_n = -\frac{Z^2}{n^2}R$$
  $R = 13.6 \text{ eV}$   $r_n = \frac{a_0}{Z}n^2$   $a_0 = 0.53 \times 10^{-10} \text{ m}$   $h\nu = E_n - E_m = Z^2 R\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$   $n > m$ 

#### The Wave Function:

 $\Psi(x,t)$  obeys Schrodinger's equation, and the normalization condition  $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$ :

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x,t)|^2 dx; \langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi(x,t) dx; \langle Q(\hat{x},\hat{p}) \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) Q\left(x, \frac{h}{i} \frac{\partial}{\partial x}\right) \Psi(x,t) dx$$

$$\tag{3}$$

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = H\Psi(x,t); \qquad \qquad \Psi(x,t) = \psi(x)e^{-iEt/\hbar}; \qquad \qquad H\psi(x) = E\psi(x)$$
 (4)

$$\rho(x,t) = |\Psi(x,t)|^2; \qquad \frac{\partial}{\partial t}\rho(\mathbf{x},t) + \nabla \cdot \mathbf{J}(\mathbf{x},t) = 0; \quad J(x,t) = \frac{i\hbar}{2m} \left(\Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x}\right)$$
(5)

$$\mathbf{J}(\mathbf{x},t) = \frac{h}{2im} \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right) \quad p = \frac{\hbar}{i} \nabla; \qquad [x_i, p_j] = i\hbar \, \delta_{i,j}$$
 (6)

Hermitian conjugate  $A^{\dagger}$  is defined by:  $\int (A\psi(x))^*\psi(x), dx = \int \psi(x)A^{\dagger}\psi(x), dx$ .

#### Fourier Transform

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int dk \Phi(k) e^{ikx}, \qquad \Phi(k) = \frac{1}{\sqrt{2\pi}} \int dx \Psi(x) e^{-ikx} \qquad \int dx |\Psi(x)|^2 = \int dk |\Phi(k)|^2 \qquad (7)$$

$$\Psi(x) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3k \Phi(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \Phi(k) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3x \Psi(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} \qquad \int d^x |\Psi(\mathbf{x})|^2 = \int d^k |\Phi(\mathbf{k})|^2 \qquad (8)$$

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dx = \delta(k) \qquad \qquad \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}} d^3x = \delta^{(3)}(k) \qquad \Psi(x,t) = \frac{1}{(2\pi)^3} \int \phi(k) e^{i(\mathbf{k}\cdot\mathbf{x}-\omega(\mathbf{k})t)} dk^3 \qquad (9)$$

#### Wavepackets

$$v_{group} = \frac{d\omega}{dk}; \ \Delta k \Delta x \simeq 1$$
 (10)

### Complete Basis Set:

Given that  $H\psi_n(x) = E_n\psi_n(x)$ ;  $\int \phi_n^*(x)\phi_n(x)dx = \delta_{nm}$ , where  $\{\phi_n\}$  is a complete set, then:

$$\psi(x) = \sum_{n} c_n \phi_n(x); \quad C_n = \int \psi_n^*(x) \psi(x) dx$$
(11)

$$\int \psi^*(x)\psi(x)dx = \sum_n |c_n|^2 = 1$$
 (12)

$$E = \int \psi_n^*(x) H \psi_m(x) dx = \sum_n |c_n|^2 E_n$$
(13)

$$\Psi(x,0) = \psi(x) = \sum_{n} c_n \phi_n(x) \implies \Psi(x,t) = \sum_{n} c_n e^{-iE_n t/\hbar} \phi_n(x)$$
 (14)

$$c_n = \int \phi_n^* \Psi(x, 0) dx \tag{15}$$

# Commutator Properties:

$$[A, A] = 0;$$
  $[A, B] = -[B, A];$   $[A + B, C] = [A, C] + [B, C]$  (16)

$$[AB, C] = [A, C]B + A[B, C]; \quad [A, BC] = [A, B]C + B[A, C];$$
 (17)

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$
(18)

# **Uncertainty Principle:**

$$(\Delta Q)^2 = \langle Q^2 \rangle - \langle Q \rangle^2 = \langle (Q - \langle Q \rangle)^2 \rangle \qquad \Delta x \Delta p \ge \frac{\hbar}{2}$$
 (19)

Where  $\Delta Q$  is the uncertainty for the Hermitian Operator Q.

#### **Operators:**

For the operator  $\hat{A}$ ,  $\hat{A}\psi=a\psi$ . a in an eigenvalue and  $\psi$  is an eigenfunction of A. Then, the following properties hold:

- $\bullet \ \hat{A}^n\psi=a^n\psi, \quad \hat{A}^{-1}\psi=a^{-1}\psi, \quad e^{i\hat{A}}\psi=e^{ia}\psi, \quad F(\hat{A})\psi=F(a)\psi$
- $\hat{A}^{\dagger} = A$ ,  $\hat{A} |\phi_n\rangle = a_n |\phi_n\rangle \implies a_n \in \mathbb{R}, \langle \phi_m | \phi_n\rangle = \delta_{mn}$
- If  $\{\phi_n\}$  is a complete and orthonormal for a Hermitian operator, then the operator is diagonal in the eigenbasis,  $\{\phi_n\}$ , with eigenvalues,,  $\{a_n\}$ , as the diagonal elements. The basis set is unique iff there are no degenerate eigenvalues.
- If two Hermitian operators,  $\hat{A}$  and  $\hat{B}$ , commute and have no degenerate eigenvalues. Then each eigenvector of  $\hat{A}$  is also an eigenvector of  $\hat{B}$ . A common orthonormal basis can be made of the joint eigenvectors of  $\hat{A}$  and  $\hat{B}$ .

#### 1D Infinite Square Well:

$$H\psi_n(x) = E_n \psi_n(x) \qquad \qquad \int \psi_n^*(x) \psi_n(x) dx = \delta_{n,m}$$
 (20)

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \qquad \qquad \phi_n(x,t) = \phi_n(x)e^{-iE_n t/\hbar}$$
(21)

$$V(x) = \begin{cases} 0, 0 \le x \le a \\ \infty, \text{ otherwise} \end{cases} \qquad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$
 (22)

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \phi_n(x) e^{-iE_n t/\hbar} \qquad c_n = \int_0^a \phi_n(x) \Psi(x,0) dx \qquad (23)$$

# Particle on a Ring:

$$\psi_{\pm}(\theta) = \frac{1}{\sqrt{2\pi}} \exp \pm i \frac{R\theta}{\hbar} \sqrt{2mE} = \frac{1}{\sqrt{2\pi}} e^{\pm ikx} \qquad x = R\theta; L = 2\pi R; k = \frac{2\pi n}{L} = \frac{n}{R}$$
 (24)

$$\psi(\theta) = \frac{1}{\sqrt{2\pi}} \exp \pm in\theta \qquad E_n = \frac{n^2 \hbar^2}{2mR^2}, \quad n = 0 \pm 1, \pm 2, \pm 3, \dots$$
 (25)

#### Harmonic Oscillator:

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m(\omega x)^2 \quad \left(\omega \equiv \sqrt{k/m}\right) \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right); n = 0, 1, 2, \dots$$
 (26)

$$H = \frac{1}{2m} [p^2 + (m\omega x)^2] = \hbar\omega \left(N + \frac{1}{2}\right) \qquad N = a_+ a_- \quad (= a^{\dagger}a)$$
 (27)

$$N\psi_n = n\psi_n \qquad N(a_+\psi_n) = [N, a_+]\psi_n \qquad (28)$$

$$[N, a_{\pm}] = \pm a_{\pm} \qquad a_{\pm} \equiv \frac{1}{\sqrt{2\hbar m\omega}} (\mp ip + m\omega x)$$
 (29)

$$x = \sqrt{\frac{\hbar}{2m\omega}} \left( a_+ + a_- \right) \qquad \qquad p = i\sqrt{\frac{m\omega\hbar}{2}} \left( a_+ - a_- \right) \tag{30}$$

$$a_{+}\psi_{n} = \sqrt{n+1}\psi_{n+1}$$
  $a_{-}\psi_{n} = \sqrt{n}\psi_{n-1}$  (31)

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \qquad \qquad \psi_n = \frac{1}{\sqrt{n!}}(a_+)^n \psi_0 \tag{32}$$

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x \qquad \mathcal{H}_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi}\right)^n e^{-\xi^2} \qquad (33)$$

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \mathcal{H}_n(\xi) e^{-\xi^2/2} \qquad \int_{-\infty}^{+\infty} \mathcal{H}_n \mathcal{H}_m e^{-x^2} dx = 2^n n! \sqrt{\pi} \delta_{n,m}$$
 (34)

### Models of Dirac Delta Distribution $\delta(x)$ :

$$\delta(x) = \lim_{\alpha \to \infty} \frac{\sin(\alpha x)}{\pi x}; \ \delta(x) = \lim_{\epsilon \to 0^+} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} e^{-\epsilon|k|} dk = \lim_{\epsilon \to 0^+} \frac{\epsilon}{\pi (x^2 + \epsilon^2)}; \ \delta(x) = \lim_{\epsilon \to 0} \frac{\Theta(x + \epsilon) - \Theta(\epsilon)}{\epsilon}$$
(35)

where  $\Theta(x)$  is Heaviside or step function.

# Bound State of Single $\delta$ -Potential:

$$V = -\alpha \delta(x), \ \alpha > 0 \qquad \qquad \psi(x) = \sqrt{\frac{m\alpha}{\hbar^2}} e^{-\frac{m\alpha}{\hbar^2}|x|} \qquad \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$
 (36)

# **Scattering State:**

$$V(x) = -\alpha \delta(x) \qquad \psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Fe^{ikx}, & x > 0 \end{cases}$$
(37)

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2} \qquad R = \frac{|B|^2}{|A|^2} = \frac{\beta}{1+\beta} \qquad (\beta = m\alpha/\hbar^2 k)$$
 (38)

#### Miscellaneous:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}; \qquad \int_{-\infty}^{\infty} e^{-(ax^2 + bx)} dx = e^{b^2/4a} \sqrt{\frac{\pi}{a}}; \qquad \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$
(39)

#### Matrix Algebra:

Let A be a 2X2 matrix defined as:  $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$  then:

$$A^{-1} = \frac{1}{|A|} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}; \qquad |A| = ad - bc \tag{40}$$

### Orbital Angular Momentum:

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \quad \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \quad \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$
 (41)

$$\left[\hat{L}_{x},\hat{L}_{y}\right]=i\hbar\hat{L}_{z},\quad\left[\hat{L}_{y},\hat{L}_{z}\right]=i\hbar\hat{L}_{x},\quad\left[\hat{L}_{z},\hat{L}_{x}\right]=i\hbar\hat{L}_{y}.\tag{42}$$

$$\hat{L}^2 \equiv \hat{L}_x \hat{L}_x + \hat{L}_y \hat{L}_y + \hat{L}_z \hat{L}_z, \quad \left[ \hat{L}^2, \hat{L}_i \right] = 0 \tag{43}$$

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}$$
 (44)

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left( \frac{\partial^2}{\partial \phi^2} \right)$$
(45)

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
(46)

$$\hat{L}^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (47)

$$\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}; \quad \hat{L}_{\pm} = \hbar e^{\pm i\phi} \left( \pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) = \hat{L}_x \pm i\hat{L}_y$$
 (48)

### General Momentum Operator

$$[J_x, J_y] = i\hbar J_z \qquad [J_z, J_x] = i\hbar J_y \qquad [J_y, J_z] = i\hbar J_x \qquad (49)$$

$$J^{2}|jm\rangle = \hbar^{2}j(j+1)|jm\rangle \qquad \qquad J_{z}|jm\rangle = \hbar m|jm\rangle \qquad \qquad J^{2} = J_{x}^{2} + J_{y}^{2} + J_{z}^{2} \qquad (50)$$

 $|jm\rangle$  are common eigenstates of the  $J^2, J_z;$ 

Thus both  $J^2$  and  $J_z$  are diagonal matrices for any fixed value of J, the dimension of these matrices is  $(2J+1)\times(2J+1)$  since  $m=-J,-J+1,\ldots,J-1,J,$  (2J+1 Values).  $J=\frac{1}{2}\implies 2J+1=$ 

 $2 \implies 2 \times 2matrices.$ 

 $J=1 \implies 2J+1=3 \implies 3 \times 3matrices.$ 

$$J_{\pm} = J_x \pm iJ_y$$
  $\sqrt{J(J+1) - m(m\pm 1)} |jm \pm 1\rangle$  (51)

so that  $J_{\pm}$  are off diagonal matrices.

We oreder the eigenvectors for a fixed J-value as the following:

$$|j,j\rangle$$
  $|j,j-1\rangle$   $|j,j-2\rangle$  ...  $|j,-j\rangle$ 

### Spin Angular Momentum Operator

For  $j = \frac{1}{2} \implies |\frac{1}{2}, \frac{1}{2}\rangle; |\frac{1}{2}, -\frac{1}{2}\rangle then:$ 

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
 (52)

$$[S_x, S_y] = i\hbar S_z \qquad [S_z, S_x] = i\hbar S_y \qquad [S_y, S_z] = i\hbar S_x \qquad (53)$$

$$S_{+} = S_x + iS_y \qquad \qquad S_{-} = S_x - iS_y \tag{54}$$

$$S_{+} = \frac{\hbar}{2} \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \qquad S_{-} = \frac{\hbar}{2} \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}$$
 (55)

### **Spherical Harmonics:**

$$Y_{\ell,m}(\theta,\phi) \equiv \mathcal{N}_{\ell,m} P_{\ell}^{m}(\cos\theta) e^{im\phi}$$
(56)

$$\hat{L}_z Y_{\ell m} = \hbar m Y_{\ell m} \tag{57}$$

$$\hat{L}^2 Y_{\ell m} = \hbar^2 \ell (\ell + 1) Y_{\ell m} \tag{58}$$

$$\int d\Omega Y_{\ell'm'}^*(\theta,\phi)Y_{\ell m}(\theta,\phi) = \delta_{\ell',\ell}\delta_{m',m}, \quad \int d\Omega = \int_0^{2\pi} d\phi \int_{-1}^1 d(\cos\theta)$$
 (59)

$$Y_{0,0}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}; \quad Y_{1,\pm 1}(\theta,\phi) = \mp \sqrt{\frac{3}{8\pi}} \sin\theta \exp(\pm i\phi); \quad Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}} \cos\theta$$
 (60)

# Central Potentials $V(\mathbf{r}) = V(r)$ :

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{61}$$

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{r} \frac{\partial^2}{\partial r^2} r - \frac{L^2(\theta, \phi)}{\hbar^2 r^2} + V(r) \right] \psi(r, \theta, \phi) = E\psi(r, \theta, \phi)$$
 (62)

$$\psi(r,\theta,\phi) = R(r)Y_{l,m} * (\theta\phi) \tag{63}$$

$$\psi(r,\theta,\phi) = \frac{u(r)}{r} Y_{\ell m}(\theta,\phi) \tag{64}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)u(r) = Eu(r)$$
(65)

$$u(r) \sim r^{\ell+1}, \text{ as } r \to 0$$
 (66)

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (67)

$$\hat{L}^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (68)

$$\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}; \quad \hat{L}_{\pm} = \hbar e^{\pm i\phi} \left( \pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) = \hat{L}_x \pm i\hat{L}_y$$
 (69)

(70)

# Hydrogen Atom (Z=1):

$$H = \frac{\mathbf{p}^2}{2m} - \frac{Ze^2}{r} \tag{71}$$

$$E_n = -\frac{Z^2 e^2}{2a_0} \frac{1}{n^2}, \quad a_0 = \frac{\hbar^2}{me^2} \simeq 0.529 \times 10^{-10} \text{ m}, \quad \frac{e^2}{2a_0} \simeq 13.6 \text{eV}$$
 (72)

$$\psi_{n,\ell,m}(\vec{x}) = A\left(\frac{r}{a_0}\right)^{\ell} \left( \text{ Polynomial in } \frac{r}{a_0} \text{ of degree } n - (\ell+1) \right) e^{-\frac{Z_r}{na_0}} Y_{\ell,m}(\theta,\phi)$$
 (73)

$$n = 1, 2, \dots, \quad \ell = 0, 1, \dots, n - 1, \quad m = -\ell, \dots, \ell$$
 (74)

$$\psi_{n,\ell,m}(\vec{x}) = \frac{u_{n\ell}(r)}{r} Y_{\ell,m}(\theta,\phi)$$
(75)

$$u_{1,0}(r) = \frac{2r}{a_0^{3/2}} \exp\left(-r/a_0\right) \tag{76}$$

$$u_{2,0}(r) = \frac{2r}{(2a_0)^{3/2}} \left( 1 - \frac{r}{2a_0} \right) \exp\left(-r/2a_0\right)$$
 (77)

$$u_{2,1}(r) = \frac{1}{\sqrt{3}} \frac{1}{(2a_0)^{3/2}} \frac{r^2}{a_0} \exp\left(-r/2a_0\right)$$
 (78)

# **Spherical Coordinates:**

$$\hat{\mathbf{r}} = \sin\theta\cos\phi\hat{\mathbf{x}} + \sin\theta\sin\phi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}}$$

$$\hat{\boldsymbol{\theta}} = \cos\theta\cos\phi\hat{\mathbf{x}} + \cos\theta\sin\phi\hat{\mathbf{y}} - \sin\theta\hat{\mathbf{z}}$$

$$\hat{\boldsymbol{\phi}} = -\sin\phi\hat{\mathbf{x}} + \cos\phi\hat{\mathbf{y}}$$

$$\hat{\mathbf{x}} = \sin\theta\cos\phi\hat{\mathbf{r}} + \cos\theta\cos\phi\hat{\boldsymbol{\theta}} - \sin\phi\hat{\boldsymbol{\phi}}$$

$$\hat{\mathbf{y}} = \sin\theta\sin\phi\hat{\mathbf{r}} + \cos\theta\sin\phi\hat{\boldsymbol{\theta}} + \cos\phi\hat{\boldsymbol{\phi}}$$

$$\hat{\mathbf{z}} = \cos\theta \hat{\mathbf{r}} - \sin\theta \hat{\boldsymbol{\theta}}$$

### **Orbital Angular Momentum:**

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \quad \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \quad \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$
 (79)

$$\left[\hat{L}_{x},\hat{L}_{y}\right]=i\hbar\hat{L}_{z},\quad\left[\hat{L}_{y},\hat{L}_{z}\right]=i\hbar\hat{L}_{x},\quad\left[\hat{L}_{z},\hat{L}_{x}\right]=i\hbar\hat{L}_{y}.\tag{80}$$

$$\hat{L}^2 \equiv \hat{L}_x \hat{L}_x + \hat{L}_y \hat{L}_y + \hat{L}_z \hat{L}_z, \quad \left[\hat{L}^2, \hat{L}_i\right] = 0$$
 (81)

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (82)

$$\hat{L}^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (83)

$$\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}; \quad \hat{L}_{\pm} = \hbar e^{\pm i\phi} \left( \pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right)$$
 (84)

# General Momentum Operator:

$$[J_x, J_y] = i\hbar J_z \qquad [J_z, J_x] = i\hbar J_y \qquad [J_y, J_z] = i\hbar J_x \qquad (85)$$

$$J^{2}|jm\rangle = \hbar^{2}j(j+1)|jm\rangle \qquad \qquad J_{z}|jm\rangle = \hbar m|jm\rangle \qquad \qquad J^{2} = J_{x}^{2} + J_{y}^{2} + J_{z}^{2}$$
 (86)

 $|jm\rangle$  are common eigenstates of the  $J^2, J_z$ ;

Thus both  $J^2$  and  $J_z$  are diagonal matrices for any fixed value of J, the dimension of these matrices is  $(2J+1)\times(2J+1)$  since  $m=-J,-J+1,\ldots,J-1,J,$  (2J+1 Values).  $J=\frac{1}{2}\implies 2J+1=2\implies 2\times 2matrices$ .

$$J=1 \implies 2J+1=3 \implies 3 \times 3matrices.$$

$$J_{\pm} = J_x \pm iJ_y$$
  $\sqrt{J(J+1) - m(m\pm 1)} |jm\pm 1\rangle$  (87)

so that  $J_{\pm}$  are off diagonal matrices.

We oreder the eigenvectors for a fixed J-value as the following:

$$|j,j\rangle$$
  $|j,j-1\rangle$   $|j,j-2\rangle$  ...  $|j,-j\rangle$ 

#### Spin Angular Momentum Operator:

For  $j = \frac{1}{2} \implies |\frac{1}{2}, \frac{1}{2}\rangle; |\frac{1}{2}, -\frac{1}{2}\rangle then:$ 

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
 (88)

$$[S_x, S_y] = i\hbar S_z \qquad [S_z, S_x] = i\hbar S_y \qquad [S_y, S_z] = i\hbar S_z \qquad (89)$$

$$[S_x, S_y] = i\hbar S_z \qquad [S_z, S_x] = i\hbar S_y \qquad [S_y, S_z] = i\hbar S_x \qquad (89)$$

$$S_+ = S_x + iS_y \qquad S_- = S_x - iS_y \qquad (90)$$

$$S_{+} = \frac{\hbar}{2} \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \qquad S_{-} = \frac{\hbar}{2} \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix} \tag{91}$$

#### **Identical Particles:**

Particles that share the same intrinsic properties: mass, charge, spin, magnetic moment, ... etc. Identical particles are indistinguishable

$$\Psi(1, 2, \dots, i, \dots, j, \dots, N) = \pm \Psi(1, 2, \dots, j, \dots, i, \dots, N)$$
(92)

are either symmetric for Bosons (integer spin particles) or antisymmetric for Fermions (half integer spin particles) under exchange of any two particles.

⇒ Pauli Exclusion Principle: Two identical Fermions cannot occupy the same quantum state.

$$\Psi_{Fermions}(R_1, R_2, \dots, R_N) = \frac{1}{\sqrt{N!}} \begin{pmatrix} \Psi_1(1) & \Psi_2(1) & \dots & \Psi_N(1) \\ \Psi_1(2) & \Psi_2(2) & \dots & \Psi_N(2) \\ \vdots & \vdots & \vdots & \vdots \\ \Psi_1(N) & \Psi_2(N) & \dots & \Psi_N(N) \end{pmatrix}$$
(93)

For Bosons use the same Slater-determinant by replacing all signs be +. Spin  $\frac{1}{2}$  particles can be in any of the following states:

Singlet State:

$$\chi_s(s1, s2) = \frac{1}{\sqrt{2}} (\chi_{\uparrow}(s1)\chi_{\downarrow}(s2) - \chi_{\downarrow}(s1)\chi_{\uparrow}(s2))$$
(94)

with total spin s=0.

Triplet States: with total spin 1, 0, -1:

$$\chi_{1,1}(s1, s2) = \chi_{\uparrow}(s1)\chi_{\uparrow}(s2)) \tag{95}$$

$$\chi_{-1,-1}(s1,s2) = \chi_{\downarrow}(s1)\chi_{\downarrow}(s2)$$
 (96)

$$\chi_{1,0}(s1, s2) = \frac{1}{\sqrt{2}} (\chi_{\uparrow}(s1)\chi_{\downarrow}(s2) + \chi_{\downarrow}(s1)\chi_{\uparrow}(s2))$$
(97)

### Electron Gas in Volume V:

Each eigenvalue in k-space occupy a volume  $\frac{2\pi^3}{V}$  so that:

$$\sum_{k} f(k) = 2 \frac{V 2\pi^3}{\int} d^3k f(k)$$
 (98)

Highest occupied wave vector is called Fermi wave vector  $k_F$ 

$$k_F = (3\pi^2 n)^{1/3}; n = \frac{N}{V} Electronic Density$$
 (99)

# Ground State of N Electrons in Volume V:

$$E_F = \frac{\hbar^2 k^2}{2m} \qquad E = 2\sum_k \frac{\hbar^2 k^2}{2m} = \frac{3}{5} N E_F$$
 (100)

$$2\frac{\Omega_k}{\frac{(2\pi)^3}{V}} = N = 2\frac{\frac{4}{3}\pi k_F^3}{\frac{(2\pi)^3}{V}}$$
  $k_F = (3\pi^2 n)^{1/3}$  (101)

$$n = \frac{N}{V} = \frac{1}{v} = \frac{1}{\frac{4}{3}\pi R_s^3}$$
 
$$R_s = \left(\frac{3}{4\pi n}\right)^{1/3}$$
 (102)

$$k_F = (3\pi^2 n)^{1/3} = \frac{(9\pi/4)^{1/3}}{R_s} = \frac{1.92}{R_s}$$
 (103)