# Formulas Sheet

# **Physical Constants:**

Quantity	Symbol, equation	Value
Speed of light	С	$2.9979 \times 10^8 \text{ m s}^{-1}$
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 > min(V(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 Schrodinger 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 are continuous all over space and in particular at the boundaries of a finite potential.
- 9. At boundaries with Dirac delta function potential, the wave function is still continuous but the first space derivative of the wavefunction is discontinuous.
- 10. Due to square integrability, 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 between adjacent states 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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$$\lambda = \frac{h}{p} = \frac{2\pi}{k} \lambda_C = \frac{h}{mc} (2)$$

# 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  $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$ :

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

$$\tag{3}$$

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = H\Psi(x,t); \qquad \Psi(x,t) = \psi(x)e^{-iEt/\hbar}; \qquad H\psi(x) = E\psi(x)$$
 (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:  $\int (A\psi(x))^*\psi(x), dx = \int \psi(x)A^{\dagger}\psi(x), dx$ .

$$H = -\frac{\hbar^2}{2m}\frac{d}{dx^2} + V(x)$$

## Fourier Transform & Wavepackets

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

$$(7)$$

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

$$(8)$$

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

$$(9)$$

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

$$\Psi(x,0) = \psi(x) = \sum_{n} c_n \phi_n(x) \implies \Psi(x,t) \begin{cases} = \sum_{n} c_n e^{-iE_n t/\hbar} \phi_n(x) \\ = e^{i\hat{H}t/\hbar} \Psi(x,0) \end{cases}$$
(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)

$$[AB, C] = [A, C]B + A[B, C]; \quad [A, BC] = [A, B]C + B[A, C]; \tag{17}$$

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$
(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.

$$(\Delta Q)^2 (\Delta R)^2 \ge \frac{1}{2} \left| \langle [Q, R] \rangle \right|^2 \tag{20}$$

## **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:

- $\hat{A}^n \psi = a^n \psi$ ,  $\hat{A}^{-1} \psi = a^{-1} \psi$ ,  $e^{i\hat{A}} \psi = e^{ia} \psi$ ,  $F(\hat{A}) \psi = F(a) \psi$
- If  $\hat{A}^{\dagger} = A$ ,  $\hat{A} |\phi_n\rangle = a_n |\phi_n\rangle \implies a_n \in \mathbb{R}, \langle \phi_m |\phi_n\rangle = \delta_{mn}$
- 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:

$$H\psi_n(x) = E_n \psi_n(x) \qquad \qquad \int \psi_n^*(x) \psi_n(x) dx = \delta_{n,m}$$
 (21)

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right); \ n = 1, 2, \dots \qquad \qquad \phi_n(x, t) = \phi_n(x)e^{-iE_nt/\hbar}$$
 (22)

$$V(x) = \begin{cases} 0, 0 \le x \le a \\ \infty, \text{ otherwise} \end{cases}$$
 
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$
 (23)

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \phi_n(x) e^{-iE_n t/\hbar} \qquad c_n = \int_0^a \phi_n(x) \Psi(x,0) dx \qquad (24)$$

## Particle on a Ring:

$$\psi_{\pm}(\theta) = \frac{1}{\sqrt{2\pi}} \exp\left(\pm i \frac{R\theta}{\hbar} \sqrt{2mE}\right) = \frac{1}{\sqrt{2\pi}} e^{\pm ikx} \qquad x = R\theta; L = 2\pi R; k = \frac{2\pi n}{L} = \frac{n}{R}$$
 (25)

$$\psi(\theta) = \frac{1}{\sqrt{2\pi}} \exp \pm in\theta \qquad E_n = \frac{n^2 \hbar^2}{2mR^2}, \quad n = 0 \pm 1, \pm 2, \pm 3, \dots$$
 (26)

#### Harmonic Oscillator:

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m(\omega x)^2 \quad \left(\omega \equiv \sqrt{k/m}\right) \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right); n = 0, 1, 2, \dots$$
 (27)

$$H = \frac{1}{2m} [p^2 + (m\omega x)^2] = \hbar\omega \left(N + \frac{1}{2}\right) \qquad N = a_+ a_- \quad (= a^{\dagger}a)$$
 (28)

$$N\psi_n = n\psi_n; \ a_{\pm} = \sqrt{\frac{m\omega}{2\hbar}} (\hat{x} \mp i\frac{\hat{p}}{m\omega}) \qquad N(a_+\psi_n) = [N, a_+]\psi_n$$
 (29)

$$[N, a_{\pm}] = \pm a_{\pm}; [a_{-}, a_{+}] = 1$$
  $a_{\pm} \equiv \frac{1}{\sqrt{2\hbar m\omega}} (\mp ip + m\omega x)$  (30)

$$x = \sqrt{\frac{\hbar}{2m\omega}} \left( a_+ + a_- \right) \qquad \qquad p = i\sqrt{\frac{m\omega\hbar}{2}} \left( a_+ - a_- \right) \tag{31}$$

$$a_{+}\psi_{n} = \sqrt{n+1}\psi_{n+1}$$
  $a_{-}\psi_{n} = \sqrt{n}\psi_{n-1}$  (32)

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \qquad \qquad \psi_n = \frac{1}{\sqrt{n!}}(a_+)^n \psi_0 \tag{33}$$

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x \qquad \mathcal{H}_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi}\right)^n e^{-\xi^2}$$
 (34)

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \mathcal{H}_n(\xi) e^{-\xi^2/2} \qquad \int_{-\infty}^{+\infty} \mathcal{H}_n \mathcal{H}_m e^{-x^2} dx = 2^n n! \sqrt{\pi} \delta_{n,m}$$
 (35)

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

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

$$(36)$$

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

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases}$$

$$(37)$$

# Bound State of Single $\delta$ -Potential: E < 0

$$V = -\alpha \delta(x), \ \alpha > 0 \qquad \qquad \psi(x) = \sqrt{\frac{m\alpha}{\hbar^2}} e^{-\frac{m\alpha}{\hbar^2}|x|} \qquad \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$
 (38)

# Scattering State: E > 0

$$V(x) = -\alpha \delta(x); k = \frac{\sqrt{2mE}}{\hbar} \qquad \psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Fe^{ikx}, & x > 0 \end{cases}$$
(39)

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2} \qquad R = \frac{|B|^2}{|A|^2} = \frac{\beta}{1+\beta} \qquad (\beta = m\alpha/\hbar^2 k)$$
 (40)

#### Miscellaneous:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}; \qquad \int_{-\infty}^{\infty} e^{-(ax^2 + bx)} dx = e^{b^2/4a} \sqrt{\frac{\pi}{a}}; \qquad \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$
(41)

# Matrix Algebra:

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

$$A^{-1} = \frac{1}{|A|} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}; |A| = ad - bc$$
 (42)

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_y = \begin{bmatrix} 0 & -1 \\ i & 0 \end{bmatrix} \qquad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$(43)$$

$$\{\sigma_i, \sigma_j\} = 2\delta_i j \qquad [\sigma_i, \sigma_j] = 2i\epsilon_{ijk} \qquad \sigma_i \sigma_j = \begin{cases} 1, & i = j \\ -\sigma_j \sigma_i, & i \neq j \end{cases}$$
 (44)

## Orbital Angular Momentum:

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \quad \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \quad \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$
 (45)

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar \hat{L}_z, \quad \left[\hat{L}_y, \hat{L}_z\right] = i\hbar \hat{L}_x, \quad \left[\hat{L}_z, \hat{L}_x\right] = i\hbar \hat{L}_y. \tag{46}$$

$$\hat{L}^2 \equiv \hat{L}_x \hat{L}_x + \hat{L}_y \hat{L}_y + \hat{L}_z \hat{L}_z, \quad \left[\hat{L}^2, \hat{L}_i\right] = 0$$
 (47)

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}$$
(48)

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left( \frac{\partial^2}{\partial \phi^2} \right)$$
(49)

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (50)

$$\hat{L}^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (51)

$$\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}; \quad \hat{L}_{\pm} = \hbar e^{\pm i\phi} \left( \pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) = \hat{L}_x \pm i\hat{L}_y$$
 (52)

# General Momentum Operator $|\vec{L}, \vec{S}, \vec{J}|$

$$[J_x, J_y] = i\hbar J_z \qquad [J_y, J_z] = i\hbar J_y \qquad [J_y, J_z] = i\hbar J_z \qquad (53)$$

$$[J_x, J_y] = i\hbar J_z \qquad [J_z, J_x] = i\hbar J_y \qquad [J_y, J_z] = i\hbar J_x \qquad (53)$$

$$J^2 |Jm\rangle = \hbar^2 j(j+1) |Jm\rangle \qquad J_z |Jm\rangle = \hbar m |Jm\rangle \qquad J^2 = J_x^2 + J_y^2 + J_z^2 \qquad (54)$$

$$J^2 = J_{\pm}J_{\mp} + J_z^2 \mp \hbar J_z \tag{55}$$

 $|Jm\rangle$  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  $m = -J, -J+1, \dots, J-1, J, (2J+1)$  Values).

$$J = \frac{1}{2} \implies 2J + 1 = 2 \implies 2 \times 2$$
 matrices.

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

$$J_{\pm} = J_x \pm iJ_y$$
  $J_{\pm} |Jm\rangle = \sqrt{J(J+1) - m(m\pm 1)} |Jm\pm 1\rangle$  (56)

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

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

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

For a fixed J here is the expectation of operator

$$A = \begin{pmatrix} \langle J|A|J\rangle & \langle J|A|J-1\rangle & \dots & \langle J|A|-J\rangle \\ \langle J-1|A|J\rangle & \langle J-1|A|J-1\rangle & \dots & \langle J-1|A|-J\rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle -J|A|J\rangle & \langle -J|A|J-1\rangle & \dots & \langle -J|A|-J\rangle \end{pmatrix}$$
(57)

in the above matrix, for a fixed J we denote  $|Jm\rangle = |m\rangle$ .

## Spin Angular Momentum Operator

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

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2} \sigma_1 \qquad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2} \sigma_2 \qquad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2} \sigma_3$$
 (58)

$$[S_x, S_y] = i\hbar S_z \qquad [S_z, S_x] = i\hbar S_y \qquad [S_y, S_z] = i\hbar S_x \qquad (59)$$

$$S_{+} = S_x + iS_y \qquad \qquad S_{-} = S_x - iS_y \tag{60}$$

$$S_{+} = \frac{\hbar}{2} \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \qquad S_{-} = \frac{\hbar}{2} \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}$$
 (61)

## **Spherical Harmonics:**

$$\langle \theta \, \phi | l \, m \rangle = Y_{\ell,m}(\theta, \phi) \equiv \mathcal{N}_{\ell,m} P_{\ell}^{m}(\cos \theta) e^{im\phi}$$
 (62)

$$\hat{L}_z Y_{\ell m} = \hbar m Y_{\ell m} \tag{63}$$

$$\hat{L}^{2}Y_{\ell m} = \hbar^{2}\ell(\ell+1)Y_{\ell m} \tag{64}$$

$$\langle l' m' | l m \rangle = \int d\Omega Y_{\ell'm'}^*(\theta, \phi) Y_{\ell m}(\theta, \phi) = \delta_{\ell', \ell} \delta_{m', m}, \quad \int d\Omega = \int_0^{2\pi} d\phi \int_{-1}^1 d(\cos \theta)$$
 (65)

$$Y_{0,0}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}; \quad Y_{1,\pm 1}(\theta,\phi) = \mp \sqrt{\frac{3}{8\pi}} \sin\theta \exp(\pm i\phi); \quad Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}} \cos\theta$$
 (66)

$$\int |\theta \, \phi\rangle \langle \theta \, \phi| \, d\Omega = 1 \qquad \sum_{lm} |l \, m\rangle \langle l \, m| = 1 \tag{67}$$

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

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$
(68)

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{r} \frac{\partial^2}{\partial r^2} r - \frac{L^2(\theta, \phi)}{\hbar^2 r^2} + V(r) \right] \psi(r, \theta, \phi) = E\psi(r, \theta, \phi)$$
 (69)

$$\psi(r,\theta,\phi) = R(r)Y_{l,m} * (\theta\phi) \tag{70}$$

$$\psi(r,\theta,\phi) = \frac{u(r)}{r} Y_{\ell m}(\theta,\phi) \tag{71}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)u(r) = Eu(r)$$
(72)

$$u(r) \sim r^{\ell+1}, \text{ as } r \to 0$$
 (73)

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_{\text{eff}}(r) \right] u(r) = E u(r); \qquad V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$
 (74)

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (75)

$$\hat{L}^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$
 (76)

$$\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}; \quad \hat{L}_{\pm} = \hbar e^{\pm i\phi} \left( \pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) = \hat{L}_x \pm i\hat{L}_y$$
 (77)

## Hydrogen Atom (Z=1):

$$V(r) = -\frac{Ze^2}{r} \qquad V_{\text{eff}}(r) = -\frac{Ze^2}{r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$
 (78)

$$H = \frac{\mathbf{p}^2}{2m} - \frac{Ze^2}{r} \tag{79}$$

$$E_n = -\frac{Z^2 e^2}{2a_0} \frac{1}{n^2}, \quad a_0 = \frac{\hbar^2}{me^2} \simeq 0.529 \times 10^{-10} \text{ m}, \quad \frac{e^2}{2a_0} \simeq 13.6 \text{eV}$$
 (80)

$$\psi_{n\ell m}(r,\theta,\phi) = A\left(\frac{r}{a_0}\right)^{\ell} \left( \text{ Polynomial in } \frac{r}{a_0} \text{ of degree } n - (\ell+1) \right) e^{-\frac{Z_r}{na_0}} Y_{\ell}^m(\theta,\phi)$$
 (81)

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell}^{m}(\theta,\phi) = \sqrt{\left(\frac{2}{na}\right)^{3} \frac{(n-\ell-1)!}{2n(n+\ell)!}} e^{\frac{-r}{na}} \left(\frac{2r}{na}\right)^{\ell} \left[L_{n-\ell-1}^{2\ell+1} \left(\frac{2r}{na}\right)\right] Y_{\ell}^{m}(\theta,\phi)$$
(82)

$$\int \psi_{n\ell m}^*(\vec{r})\psi_{n'\ell'm'}(\vec{r})d^3\vec{r} = \delta_{nn'}\delta_{mm'}\delta_{\ell\ell'}$$
(83)

$$\hat{H}\psi_{n\ell m}(\vec{r}) = E_n \psi_{n\ell m}(\vec{r}) \tag{84}$$

$$n = 1, 2, \dots, \quad \ell = 0, 1, \dots, n - 1, \quad m = -\ell, \dots, \ell$$
 (85)

$$\psi_{n\ell m}(r,\theta,\phi) = \frac{u_{n\ell}(r)}{r} Y_{\ell}^{m}(\theta,\phi)$$
(86)

$$u_{1,0}(r) = \frac{2r}{a_0^{3/2}} \exp\left(-r/a_0\right) \tag{87}$$

$$u_{2,0}(r) = \frac{2r}{(2a_0)^{3/2}} \left( 1 - \frac{r}{2a_0} \right) \exp\left( -r/2a_0 \right)$$
(88)

$$u_{2,1}(r) = \frac{1}{\sqrt{3}} \frac{1}{(2a_0)^{3/2}} \frac{r^2}{a_0} \exp(-r/2a_0)$$
(89)

$$\Psi_{100}(r,\theta,\phi) = \frac{2r}{\sqrt{4\pi a_0^3}} e^{-r/a_0} \tag{90}$$

### Transfer Matrix

$$\begin{bmatrix} F \\ G \end{bmatrix} = M \begin{bmatrix} A \\ B \end{bmatrix} \qquad M = \begin{bmatrix} M_{11} & M_{12} \\ M_{12}^* & M_{11}^* \end{bmatrix} \qquad \det M = 1 \tag{91}$$

$$T = \frac{1}{|M_{22}|^2}; \qquad R + T = 1 \tag{92}$$

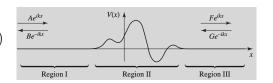


Figure 1: Scattering from an arbitrary localized potential (V(x) = 0 except for Region II)

## **Spherical Coordinates:**

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

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

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

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

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

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

#### **Identical Particles:**

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

$$\Psi(1, 2, \dots, i, \dots, j, \dots, N) = \pm \Psi(1, 2, \dots, j, \dots, i, \dots, N)$$
(93)

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.

$$\Psi_{Fermions}(R_1, R_2, \dots, R_N) = \frac{1}{\sqrt{N!}} \begin{pmatrix} \Psi_1(R_1) & \Psi_2(R_1) & \dots & \Psi_N(R_1) \\ \Psi_1(R_2) & \Psi_2(R_2) & \dots & \Psi_N(R_2) \\ \vdots & \vdots & \vdots & \vdots \\ \Psi_1(R_N) & \Psi_2(R_N) & \dots & \Psi_N(R_N) \end{pmatrix}$$
(94)

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 (Antisymmetric state):

$$\chi_s(s1, s2) = \frac{1}{\sqrt{2}} (\chi_{\uparrow}(s1)\chi_{\downarrow}(s2) - \chi_{\downarrow}(s1)\chi_{\uparrow}(s2)) \tag{95}$$

with total spin s=0.

Triplet States (Symmetric state): with total spin  $S_z=1,\,0,\,$ -1:

$$\chi_{T}(s_{1}, s_{2}) \begin{cases}
\chi_{1,1}(s_{1}, s_{2}) = \chi_{\uparrow}(s_{1})\chi_{\uparrow}(s_{2}) \\
\chi_{-1,-1}(s_{1}, s_{2}) = \chi_{\downarrow}(s_{1})\chi_{\downarrow}(s_{2}) \\
\chi_{1,0}(s_{1}, s_{2}) = \frac{1}{\sqrt{2}}(\chi_{\uparrow}(s_{1})\chi_{\downarrow}(s_{2}) + \chi_{\downarrow}(s_{1})\chi_{\uparrow}(s_{2}))
\end{cases} (96)$$

## Electron Gas in Volume V:

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

$$\sum_{k} f(k) = 2\frac{V}{(2\pi)^3} \int d^3k f(k)$$
 (97)

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 (98)

## Ground State of N Electrons in Volume V:

$$E_F = \frac{\hbar^2 k^2}{2m} \qquad E = 2\sum_k \frac{\hbar^2 k^2}{2m} = \frac{3}{5} N E_F \tag{99}$$

$$2\frac{\Omega_k}{\frac{(2\pi)^3}{V}} = N = 2\frac{\frac{4}{3}\pi k_F^3}{\frac{(2\pi)^3}{V}}$$
  $k_F = (3\pi^2 n)^{1/3}$  (100)

$$n = \frac{N}{V} = \frac{1}{v} = \frac{1}{\frac{4}{3}\pi r_s^3}$$
  $r_s = \left(\frac{3}{4\pi n}\right)^{1/3}$  (101)

$$k_F = (3\pi^2 n)^{1/3} = \frac{(9\pi/4)^{1/3}}{r_s} = \frac{1.92}{r_s}$$
 (102)

### Bloch Theorem in Solids:

$$\psi(R+x) = e^{ik \cdot R} \psi(x) \tag{103}$$

In 3D: 
$$k_i = \frac{2\pi n_i}{L}$$
;  $i = x, y, z$ ;  $n = 0, \pm 1, \pm 2, ... \Rightarrow dn = \frac{V}{(2\pi)^3} dk^3$  (104)

$$\sum_{k\sigma} F(k,\sigma) = \frac{V}{(2\pi)^3} \sum_{\sigma} \int dk^3 F(k,\sigma)$$
 (105)

## Probability Distributions:

We have three distributions, one for classical particles (Maxwell-Boltzmann) and two for undistinguishable particles (Fermi-Dirac for fermions and Bose-Einstein for bosons). Their equations are the following:

$$P(E) = \frac{1}{e^{\beta(E - E_f)} + 1}$$
 Fermi-Dirac Dist. (106)

$$e^{\beta(E-E_f)} + 1$$

$$P(E) = \frac{1}{e^{\beta(E-\mu)} - 1} \quad \text{Bose-Einstein Dist.}$$

$$P(E) = \frac{1}{e^{\beta(E-\mu)}} \quad \text{Maxwell-Boltzmann Dist.}$$

$$(107)$$

$$P(E) = \frac{1}{e^{\beta(E-\mu)}}$$
 Maxwell-Boltzmann Dist. (108)

Where 
$$\beta = \frac{1}{k_B T}$$
 (109)

The plots of these distributions for different temperatures:

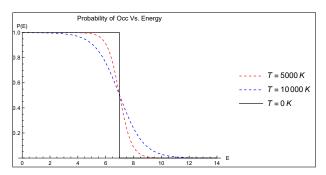


Figure 1: Fermi–Dirac Dist. when  $E_f = 7eV$ . For fermions

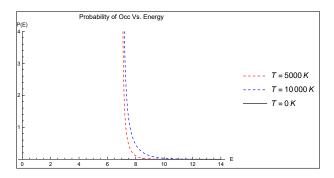
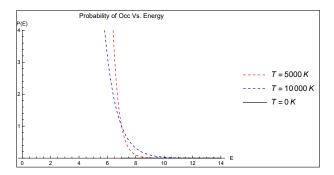


Figure 2: Bose–Einstein Dist. when  $\mu = 7eV$ . For bosons



**Figure 3:** Maxwell–Boltzmann Dist. when  $\mu = 7eV$ . For bosons

## Non-Degenerate Perturbation Theory

$$H = H^0 + \lambda H' = H(\lambda) \tag{110}$$

$$H(\lambda)\psi_n(\lambda) = E_n(\lambda)\psi_n(\lambda) \tag{111}$$

$$\psi_n(\lambda) = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \cdots$$
(112)

$$E_n(\lambda) = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots$$
(113)

Assume 
$$\psi_n(\lambda)$$
,  $E_n(\lambda)$  converges (114)

(115)

$$\lambda^0: \quad H^0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle \tag{116}$$

$$\lambda^{1}: \quad H^{0}|\psi_{n}^{1}\rangle + H'\psi_{n}^{0} = E_{n}^{0}|\psi_{n}^{1}\rangle + E_{n}^{1}|\psi_{n}^{0}\rangle \tag{117}$$

$$\lambda^{2}: H^{0}|\psi_{n}^{2}\rangle + H'\psi_{n}^{1} = E_{n}^{0}|\psi_{n}^{2}\rangle + E_{n}^{1}|\psi_{n}^{1}\rangle + E_{n}^{2}|\psi_{n}^{0}\rangle$$
(118)

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle \tag{119}$$

$$|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0 \rangle \tag{120}$$

$$E_n^2 = \langle \psi_n^0 | H' | \psi_n^1 \rangle \tag{121}$$

$$E_n^2 = \sum_{m \neq n} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}$$
 (122)

Let  $|\psi_1^0\rangle$  and  $|\psi_2^0\rangle$  be degenerate states of  $H^0$ , then

$$H' = \begin{bmatrix} H'_{11} & H'_{12} \\ H'_{21} & H'_{22} \end{bmatrix}; \quad \text{where} \quad H'_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle$$
 (123)

$$|H' - E^{1}I| = \begin{bmatrix} H'_{11} - E^{1} & H'_{12} \\ H'_{21} & H'_{22} - E^{1} \end{bmatrix} \begin{bmatrix} \alpha_{1} \\ \alpha_{2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
 (124)

$$E_{\pm}^{1} = \frac{1}{2} \left[ H'_{11} + H'_{22} \pm \sqrt{(H'_{11} - H'_{11})^{2} + 4|H'_{12}|^{2}} \right] \quad \text{and} \quad |\psi_{\pm}\rangle = \alpha_{1}|\psi_{1}^{0}\rangle + \alpha_{2}|\psi_{2}^{0}\rangle$$
 (125)