

Formulas Sheet

Physical Constants:

Quantity	Symbol, equation	Value
Speed of light	c	$2.9979 \times 10^8 \text{ m s}^{-1}$
Electron charge	e	$1.602 \times 10^{-19} \text{ C}$
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	$\hbar c$	$197.327 \text{ MeV fm} = 197.327 \text{ eV nm}$
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	$\mathcal{R} = m_e c^2 \alpha^2/2$	$13.606 \text{ eV}^{-11} \text{ MeV T}^{-1}$
Bohr magneton	$\mu_B = e\hbar/2m_e$	5.788×10^{-11}
Nuclear magneton	$\mu_N = e\hbar/2m_p$	$3.152 \times 10^{-14} \text{ MeV T}^{-1}$
Avogadro number	N_A	$6.022 \times 10^{23} \text{ mol}^{-1}$
Boltzmann constant	k	$1.381 \times 10^{-23} \text{ J K}^{-1}$ $= 8.617 \times 10^{-5} \text{ eV K}^{-1}$
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	$\epsilon_0 = 1/\mu_0 c^2$	$8.854 \times 10^{-12} \text{ F m}^{-1}$
Permeability of free space	μ_0	$4\pi \times 10^{-7} \text{ N A}^{-2}$

Conversion of units:

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

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 overall 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:

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

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

Blackbody Radiation:

Planck 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.

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

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

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

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x, t)|^2 dx; \quad \langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi(x, t) dx; \quad \langle Q(\hat{x}, \hat{p}) \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) Q \left(x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi(x, t) dx \quad (3)$$

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

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

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

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

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

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

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

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

Complete Basis Set:

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

$$\psi(x) = \sum_n c_n \phi_n(x); \quad c_n = \int \psi_n^*(x) \psi(x) dx \quad (11)$$

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

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

$$\Psi(x, 0) = \psi(x) = \sum_n c_n \phi_n(x) \implies \Psi(x, t) \begin{cases} = \sum_n c_n e^{-iE_n t/\hbar} \phi_n(x) \\ = e^{i\hat{H}t/\hbar} \Psi(x, 0) \end{cases} \quad (14)$$

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

Commutator Properties:

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

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

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

Uncertainty Principle:

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

Where ΔQ is the uncertainty for the Hermitian Operator Q .

$$(\Delta Q)^2 (\Delta R)^2 \geq \frac{1}{2} |\langle [Q, R] \rangle|^2 \quad (20)$$

Operators:

For the operator \hat{A} , $\hat{A}\psi = a\psi$. a is an eigenvalue and ψ 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 $\hat{A}^\dagger = \hat{A}$, $\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle \implies a_n \in \mathbb{R}$, $\langle \phi_m | \phi_n \rangle = \delta_{mn}$
- 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:

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

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

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

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

Particle on a Ring:

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

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

Harmonic Oscillator:

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

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

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

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

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

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

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

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

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

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

$$\delta(x) = \lim_{\alpha \rightarrow \infty} \frac{\sin(\alpha x)}{\pi x}; \delta(x) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} e^{-\epsilon|k|} dk = \lim_{\epsilon \rightarrow 0^+} \frac{\epsilon}{\pi(x^2 + \epsilon^2)}; \delta(x) = \lim_{\epsilon \rightarrow 0} \frac{\Theta(x + \epsilon) - \Theta(\epsilon)}{\epsilon} \quad (36)$$

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

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} \quad (37)$$

Bound State of Single δ -Potential: $E < 0$

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

Scattering State: $E > 0$

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

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

Miscellaneous:

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

Matrix Algebra:

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

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

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -1 \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (43)$$

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij} \quad [\sigma_i, \sigma_j] = 2i \in ijk \quad \sigma_i \sigma_j = \begin{cases} 1, & i = j \\ -\sigma_j \sigma_i, & i \neq j \end{cases} \quad (44)$$

Orbital Angular Momentum:

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

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y. \quad (46)$$

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

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

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

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

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

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

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

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

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

$$J^2 = J_{\pm} J_{\mp} + J_z^2 \mp \hbar J_z \quad (55)$$

$|Jm\rangle$ 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).

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

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

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

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

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

$$|J, J\rangle \quad |J, J-1\rangle \quad |J, J-2\rangle \quad \dots \quad |J, -J\rangle$$

For a fixed J here is the expectation of operator A:

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

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 :

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

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

$$S_+ = S_x + iS_y \quad S_- = S_x - iS_y \quad (60)$$

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

Spherical Harmonics:

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

$$\hat{L}_z Y_{\ell m} = \hbar m Y_{\ell m} \quad (63)$$

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

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

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

$$\int |\theta \phi\rangle \langle \theta \phi| d\Omega = 1 \quad \sum_{lm} |l m\rangle \langle l m| = 1 \quad (67)$$

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

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

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

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

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

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

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

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

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

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

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

Hydrogen Atom (Z=1):

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

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

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

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

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

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

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

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

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

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

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

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

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

Transfer Matrix

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

$$T = \frac{1}{|M_{22}|^2}; \quad R + T = 1 \quad (92)$$

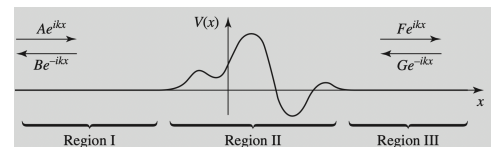


Figure 1: Scattering from an arbitrary localized potential ($V(x) = 0$ except for Region II)

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

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

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

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

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

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):

$$\chi_s(s_1, s_2) = \frac{1}{\sqrt{2}}(\chi_{\uparrow}(s_1)\chi_{\downarrow}(s_2) - \chi_{\downarrow}(s_1)\chi_{\uparrow}(s_2)) \quad (95)$$

with total spin $s=0$.

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

$$\chi_T(s_1, s_2) \begin{cases} \chi_{1,1}(s_1, s_2) = \chi_{\uparrow}(s_1)\chi_{\uparrow}(s_2) \\ \chi_{-1,-1}(s_1, s_2) = \chi_{\downarrow}(s_1)\chi_{\downarrow}(s_2) \\ \chi_{1,0}(s_1, s_2) = \frac{1}{\sqrt{2}}(\chi_{\uparrow}(s_1)\chi_{\downarrow}(s_2) + \chi_{\downarrow}(s_1)\chi_{\uparrow}(s_2)) \end{cases} \quad (96)$$

Electron Gas in Volume V:

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

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

Highest occupied wave vector is called Fermi wave vector k_F

$$k_F = (3\pi^2 n)^{1/3}; \quad n = \frac{N}{V} \text{ Electronic Density} \quad (98)$$

Ground State of N Electrons in Volume V:

$$E_F = \frac{\hbar^2 k^2}{2m} \quad E = 2 \sum_k \frac{\hbar^2 k^2}{2m} = \frac{3}{5} N E_F \quad (99)$$

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

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

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

Bloch Theorem in Solids:

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

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

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

Probability Distributions:

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

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

$$P(E) = \frac{1}{e^{\beta(E-\mu)} - 1} \quad \text{Bose-Einstein Dist.} \quad (107)$$

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

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

The plots of these distributions for different temperatures:

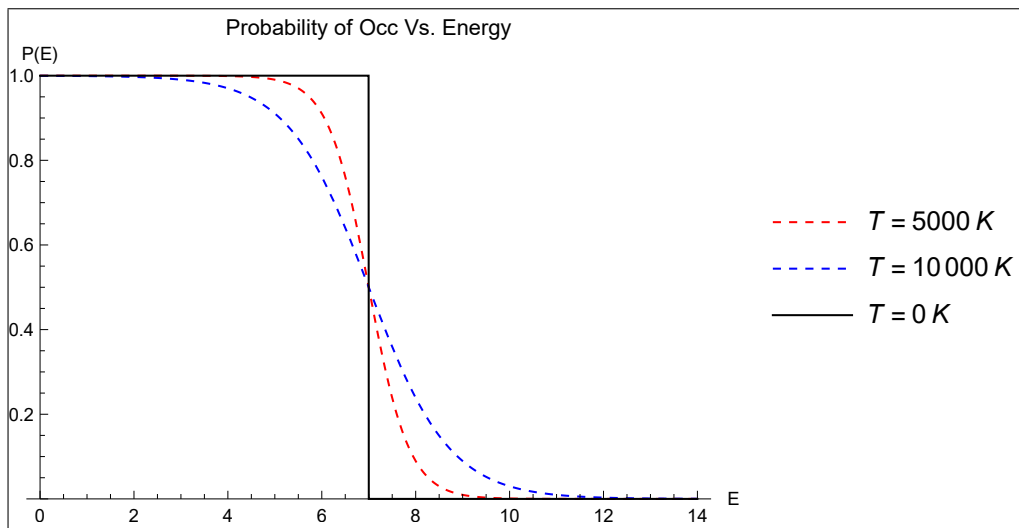


Figure 1: Fermi–Dirac Dist. when $E_f = 7 \text{ eV}$. For fermions

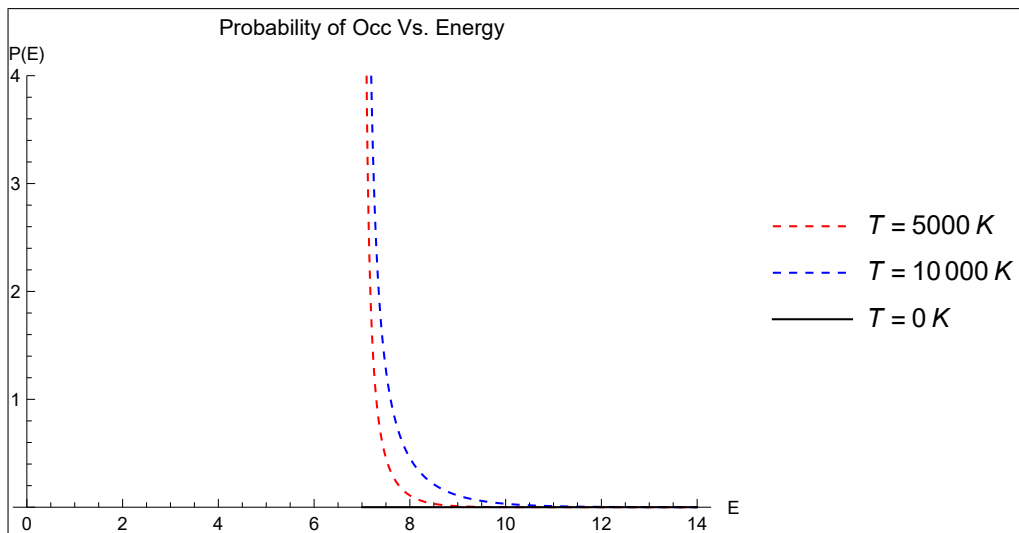


Figure 2: Bose–Einstein Dist. when $\mu = 7 \text{ eV}$. For bosons

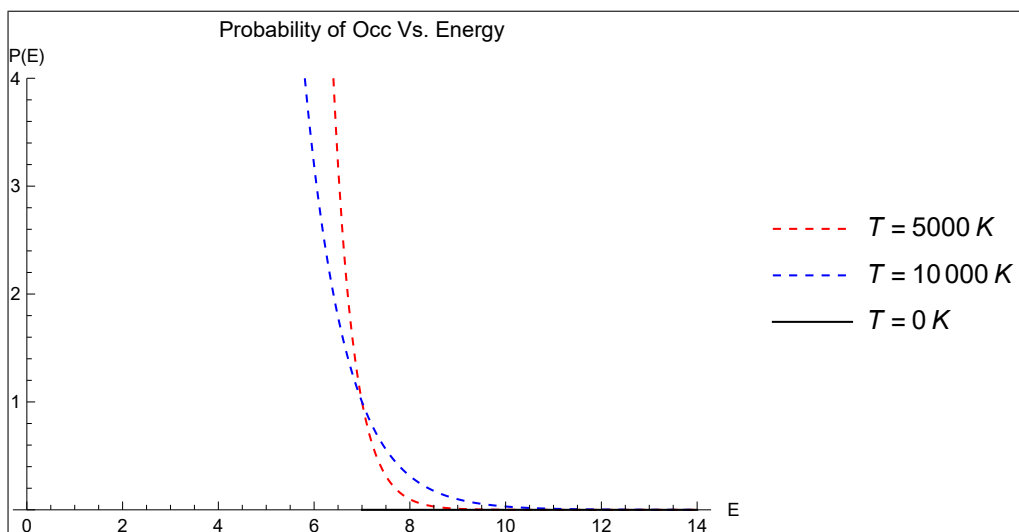


Figure 3: Maxwell–Boltzmann Dist. when $\mu = 7 \text{ eV}$. For bosons

Non-Degenerate Perturbation Theory

$$H = H^0 + \lambda H' = H(\lambda) \quad (110)$$

$$H(\lambda)\psi_n(\lambda) = E_n(\lambda)\psi_n(\lambda) \quad (111)$$

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

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

$$\text{Assume } \psi_n(\lambda), E_n(\lambda) \text{ converges} \quad (114)$$

$$(115)$$

$$\lambda^0 : H^0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle \quad (116)$$

$$\lambda^1 : H^0|\psi_n^1\rangle + H'\psi_n^0 = E_n^0|\psi_n^1\rangle + E_n^1|\psi_n^0\rangle \quad (117)$$

$$\lambda^2 : H^0|\psi_n^2\rangle + H'\psi_n^1 = E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle \quad (118)$$

$$E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle \quad (119)$$

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

$$E_n^2 = \langle\psi_n^0|H'|\psi_n^1\rangle \quad (121)$$

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

Degenerate Perturbation Theory

For 2-fold degeneracy

$$\begin{pmatrix} H'_{11} - E^1 & H'_{12} \\ H'_{21} & H'_{22} - E^1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = 0$$

with eigenenergies

$$E_{\pm}^1 = \frac{1}{2} \left(H'_{11} + H'_{22} \pm \sqrt{(H'_{11} - H'_{22})^2 + 4|H'_{12}|^2} \right)$$

and eigenfunctions $|\psi_{\pm}^0\rangle = \alpha_1|\psi_1^0\rangle + \alpha_2|\psi_2^0\rangle$. Which should be normalized.

For n-fold degeneracy

$$H' \vec{\alpha} = E_m^1 \vec{\alpha}$$

$$\Rightarrow \sum_{j=1}^n (H'_{ij} - E_m^1 \delta_{ij}) \alpha_j = 0, \quad \text{for } i = 1, 2, \dots, n$$

where $1 \leq m \leq n$, H' is an $n \times n$ matrix. And

$$\vec{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_n)^\top$$

$$H^0 |\psi_i^0\rangle = E_i^0 |\psi_i^0\rangle$$

$$H'_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle$$

$$|\psi^0\rangle = \sum_{i=1}^n \alpha_i |\psi_i^0\rangle$$

$$H(\lambda) = H^0 + \lambda H'$$

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

$$|\psi_n(\lambda)\rangle = |\psi_n^0\rangle + \lambda |\psi_n^1\rangle + \lambda^2 |\psi_n^2\rangle + \dots$$