QUANTUM MECHANICS FORMULA SHEET

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1.Wave Particle Duality

1.1 De Broglie Wavelengths

The wavelength of the wave associated with a particle is given by the de Broglie relation

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$ where h is Plank's constant

For relativistic case, the mass becomes $m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$ where m_0 is rest mass and v is velocity of body.

1.2 Heisenberg's Uncertainty Principle

"It is impossible to determine two canonical variables simultaneously for microscopic particle". If q and p_q are two canonical variable then

$$\Delta q \Delta p_q \geq \frac{\hbar}{2}$$

where Δq is the error in measurement of q and Δp_q is error in measurement of p_q and h is Planck's constant $(\hbar \equiv h/2\pi)$.

Important uncertainty relations

- $\Delta x \cdot \Delta P_x \geq \frac{\hbar}{2}$ (x is position and p_x is momentum in x direction)
- $\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$ (E is energy and t is time).
- $\Delta L \cdot \Delta \theta \geq \frac{\hbar}{2}$ (L is angular momentum, θ is angle measured)

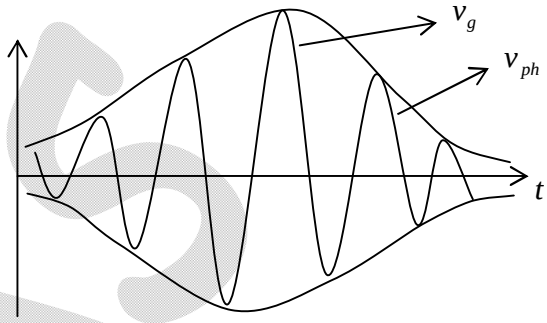
1.3 Group Velocity and Phase Velocity

According to de Broglie, matter waves are associated with every moving body. These matter waves moves in a group of different waves having slightly different wavelengths. The formation of group is due to superposition of individual wave.

Let If $\psi_1(x,t)$ and $\psi_2(x,t)$ are two waves of slightly different wavelength and frequency.

$$\psi_1 = A\sin(kx-\omega t), \qquad \psi_2 = A\sin[(k+dk)x-(\omega+d\omega)t]$$

$$\psi = \psi_1+\psi_2 = 2A\cos\left(\frac{dk}{2}-\frac{d\omega t}{2}\right)\sin(kx-\omega t)$$



The velocity of individual wave is known as Phase velocity which is given as $v_p = \frac{\omega}{k}$. The velocity of amplitude is given by group velocity v_g i.e. $v_g = \frac{d\omega}{dk}$

The relationship between group and phase velocity is given by

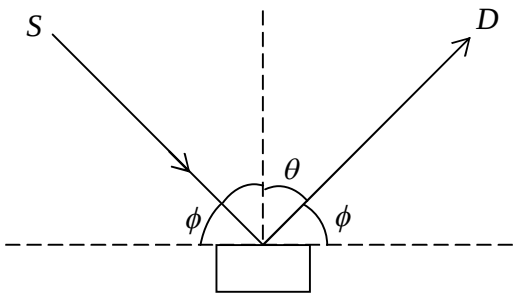
$$v_g = \frac{d\omega}{dk} = v_p + k\frac{dv_p}{dk};\ v_g = v_p - \lambda\frac{dv_p}{d\lambda}$$

Due to superposition of different wave of slightly different wavelength resultant wave moves like a wave packet with velocity equal to group velocity.

1.4 Experimental evidence of wave particle duality

1.4.1 Wave nature of particle (Davisson-German experiment)

Electron strikes the crystals surface at an angle ϕ. The detector, symmetrically located from the source measure the number of electrons scattered at angle θ where θ is the angle between incident and scattered electron beam.



The Maxima condition is given by $n\lambda = 2d\sin\phi$

$or\ n\lambda = 2d\cos\left(\frac{\theta}{2}\right)$ where $\lambda = \frac{h}{p}$

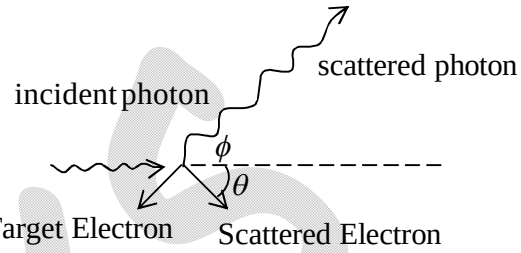
1.4.2 Particle nature of wave (Compton and Photoelectric Effect)

Compton Effect

The Compton Effect is the result of scattering of a photon by an electron. Energy and momentum are conserved in such an event and as a result the scattered photon has less energy (longer wavelength) then the incident photon.

If λ is incoming wavelength and λ' is scattered wavelength and ϕ is the angle made by scattered wave to the incident wave then

$$\lambda' - \lambda = \frac{h}{m_o c}(1 - \cos\phi)$$



where $\frac{h}{m_o c}$ known as λ_c which is Compton wavelength (λ_c = 2.426 x 10^{-12} m) and m_o is rest mass of electron.

Photoelectric effect

When a metal is irradiated with light, electron may get emitted. Kinetic energy k of electron leaving when irradiated with a light of frequency $\nu > \nu_o$, where ν_o is threshold frequency. Kinetic energy is given by

$$k_{\max} = h\nu - h\nu_0$$

Stopping potential V_s is potential required to stop electron which contain maximum kinetic energy $(k_{\max})$.

$eV_s = h\nu - h\nu_0$, which is known as Einstein equation

2. Mathematical Tools for Quantum Mechanics

2.1 Dimension and Basis of a Vector Space

A set of N vectors $\phi_1, \phi_2, ...\phi_N$ is said to be linearly independent if and only if the solution of equation $\sum_{i=1}^{N} a_i \phi_i = 0$ is $a_1 = a_2 = ... a_N = 0$

N dimensional vector space can be represent as $\psi = \sum_{i=1}^{N} a_i \phi_i = 0$ where i = 1, 2, 3 … are linearly independent function or vector.

Scalar Product: Scalar product of two functions is represented as (ϕ, ψ), which is defined as $\int \phi^* \psi \, dx$. If the integral diverges scalar product is not defined.

Square Integrable: If the integration or scalar product $(\psi, \psi) = \int |\psi|^2 \, dx$ is finite then the integration is known as square integrable.

Dirac Notation: Any state vector ψ can be represented as $|\psi\rangle$ which is termed as *ket* and conjugate of ψ i.e. ψ^* is represented by $\langle\psi|$ which is termed as *bra*.

The scalar product of ϕ and ψ in Dirac Notation is represented by $\langle\phi|\psi\rangle$ (*bra-ket*). The value of $\langle\phi|\psi\rangle$ is given by integral $\int \phi^*(r,t)\psi(r,t) d^3r$ in three dimensions.

Properties of kets, bras and brakets:

$$(a|\psi\rangle)^* = a^* \langle\psi|$$
$$\langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle$$

Orthogonality relation: If $|\psi\rangle$ and $|\phi\rangle$ are two ket and the value of bracket $\langle\psi|\phi\rangle = 0$ then $|\psi\rangle$, $|\phi\rangle$ is orthogonal.

Orthonormality relation: If $|\psi\rangle$ and $|\phi\rangle$ are two ket and the value of bracket $\langle\psi|\phi\rangle = 0$ and $\langle\psi|\psi\rangle = 1$ $\langle\phi|\phi\rangle = 1$ then $|\psi\rangle$ and $|\phi\rangle$ are orthonormal.

Schwarz inequality: $|\langle\psi|\phi\rangle|^2 \le \langle\psi|\psi\rangle\langle\phi|\phi\rangle$

2.2 Operators

An operator A is mathematical rule that when applied to a *ket* $|\phi\rangle$ transforms it into another ket $|\psi\rangle$ i.e.

$$A|\phi\rangle = |\psi\rangle$$

Different type of operator

Identity operator $I|\psi\rangle = |\psi\rangle$

Parity operator $\pi|\psi(r)\rangle = |\psi(-r)\rangle$

For even parity $\pi|\psi(r)\rangle = |\psi(r)\rangle$, for odd parity $\pi|\psi(r)\rangle = -|\psi(r)\rangle$

Momentum operator $P_x|\psi\rangle = -i\hbar\dfrac{\partial|\psi\rangle}{\partial x}$

Energy operator $H|\psi\rangle = i\hbar\dfrac{\partial|\psi\rangle}{\partial\ t}$

Laplacian operator $\nabla^2|\psi\rangle = \dfrac{\partial^2|\psi\rangle}{\partial x^2} + \dfrac{\partial^2|\psi\rangle}{\partial y^2} + \dfrac{\partial^2|\psi\rangle}{\partial z^2}$

Position operator $X|\psi(r)\rangle = x|\psi(r)\rangle$

Linear operator

For $|\psi\rangle = a_1|\phi_1\rangle + a_2|\phi_2\rangle$ if an operator $\hat{A}$ applied on $|\psi\rangle$ results in $a_1A|\phi_1\rangle + a_2A|\phi_2\rangle$ then operator $\hat{A}$ is said to be linear operator.

2.3 Postulates of Quantum Mechanics

Postulate 1: State of system

The state of any physical system is specified at each time t by a state vector $|\psi(t)\rangle$ which contains all the information about the system. The state vector is also referred as wave function. The wave function must be: Single valued, Continuous, Differentiable, Square integrable (i.e. wave function have to converse at infinity).

Postulate 2: To every physically measurable quantity called as observable dynamical variable. For every observable there corresponds a linear Hermitian operator $\hat{A}$. The Eigen vector of $\hat{A}$ let say $|\phi_n\rangle$ form complete basis. Completeness relation is given by $\sum_{n=1}^{\infty}|\phi_n\rangle\langle\phi_n| = I$

Eigen value: The only possible result of measurement of a physical quantity a_n is one of the Eigen values of the corresponding observable.

Postulate 3: (Probabilistic outcome): When the physical quantity A is measured on a system in the normalized state $|\psi\rangle$ the probability P(a_n) of obtaining the Eigen value a_n of corresponding observable A is $P(a_n) = \frac{\sum_{i=1}^{g_n}\left|\langle a_n^i|\psi\rangle\right|^2}{\langle\psi|\psi\rangle}$ where g_n is degeneracy of state and $|u_n\rangle$ is the Normalised Eigen vector of $\hat{A}$ associated with Eigen value a_n.

Postulate 4: Immediately after measurement.

If the measurement of physical quantity A on the system in the state $|\psi\rangle$ gives the result a_n (a_n is Eigen value associated with Eigen vector $|a_n\rangle$), Then the state of the system immediately after the measurement is the normalized projection $\frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}}$ where P_n is projection operator defined by $|\phi_n\rangle\langle\phi_n|$.

Projection operator $\hat{P}$: An operator $\hat{P}$ is said to be a projector, or projection operator, if it is Hermitian and equal to its own square i.e. $\hat{P}^2 = \hat{P}$

The projection operator is represented by $\sum_n |\phi_n\rangle\langle\phi_n|$

Postulate 5: The time evolution of the state vector $|\psi(t)\rangle$ is governed by Schrodinger equation: $i\hbar\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$, where *H(t)* is the observable associated with total energy of system and popularly known as Hamiltonian of system. Some other operator related to quantum mechanics:

2.4 Commutator

If A and B are two operator then their commutator is defined as $[A,B] = AB\text{-}BA$

Properties of commutators

$[A,B] = -[B,A]$; $\quad [A,B+C] = [A,B]+[A,C]$

$[A,BC] = [A,B]C + B[A,C]$; $\quad [A,B]^{\dagger} = [B^{\dagger},A^{\dagger}]$

$[A,[B,C]]+[B[C,A]]+[C,[A,B]] = 0$ (Popularly known as Jacobi identity).

$[A, f(A)] = 0$

If X is position and P_x is conjugate momentum then

$[X^n, P_x] = nX^{n-1}(i\hbar)$ and $[X, P_x^n = nP_x^{n-1}(i\hbar)]$

If b is scalar and A is any operator then $[A,b] = 0$

If [A, B] = 0 then it is said that A and B commutes to each other ie $AB = BA$.

If two Hermition operators A and B, commute ie $[A,B] = AB - BA = 0$ and if A has non degenerate Eigen value, then each Eigen vector of $\hat{A}$ is also an Eigen vector of B.

We can also construct the common orthonormal basis that will be joint Eigen state of A and B.

The anti commutator is defined as $[A,B] = AB + BA$

2.5 Eigen value problem in Quantum Mechanics

Eigen value problem in quantum mechanics is defined as

$$\mathrm{A}|\phi_n\rangle = a_n|\phi_n\rangle$$

where a_n is Eigen value and $|\phi_n\rangle$ is Eigen vector.

- In quantum mechanics operator associated with observable is Hermitian, so its Eigen values are real and Eigen vector corresponding to different Eigen values are orthogonal.
- The Eigen state (Eigen vector) of Hamilton operator defines a complete set of mutually orthonormal basis state. This basis will be unique if Eigen value are non degenerate and not unique if there are degeneracy.

Completeness relation: the orthonormnal realtion and completeness relation is given by

$$\langle\phi_n|\phi_m\rangle = \delta_{mn}, \qquad \sum_{n=1}^{\infty}|\phi_n\rangle\langle\phi_n| = I$$

where I is unity operator.

2.6 Time evaluation of the expectation of A (Ehrenfest theorem)

$\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle[\mathrm{A,H}]\rangle + \left\langle\frac{\partial \mathrm{A}}{\partial t}\right\rangle$ where $[A,H]$ is commutation between operator A and Hamiltonian H operator .Time evaluation of expectation of A gives rise to Ehrenfest theorem .

$$\frac{d}{dt}\langle R\rangle = \frac{1}{m}\langle P\rangle \ , \ \frac{d}{dt}\langle P\rangle = -\langle\nabla V(R,t)\rangle$$

where R is position, P is momentum and $V(R,t)$ is potential operator.

2.7 Uncertainty relation related to operator

If $\hat{\mathrm{A}}$ and $\hat{\mathrm{B}}$ are two operator related to observable A and B then

$$\Delta\hat{\mathrm{A}}\,\Delta\hat{\mathrm{B}} \geq \frac{1}{2}\left|\left\langle\left[\hat{\mathrm{A}},\hat{\mathrm{B}}\right]\right\rangle\right|$$

where $\Delta\hat{\mathrm{A}} = \sqrt{\langle\hat{\mathrm{A}}^2\rangle - \langle\hat{\mathrm{A}}\rangle^2}$ and $\Delta\hat{\mathrm{A}} = \sqrt{\langle\hat{\mathrm{B}}^2\rangle - \langle\hat{\mathrm{B}}\rangle^2}$.

2.8 Change in basis in quantum mechanics

If $\psi(k)$ are wave function is position representation and $\phi(k)$ are wave function in momentum representation, one can change position to momentum basis via Fourier transformation.

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi\ (x) e^{-ikx} dx$$

2.9 Expectation value and uncertainty principle

The expectation value $\langle A \rangle$ of A in direction of $|\psi\rangle$ is given by

$$\langle A \rangle = \frac{\langle \psi | A | \psi \rangle}{\langle \psi | \psi \rangle} \text{ or}$$

$\langle A \rangle = \sum a_n P_n$ where P_n is probability to getting Eigen value a_n in state $|\psi\rangle$.

3. Schrödinger Wave Equation and Potential Problems

3.1 Schrödinger Wave Equation

Hamiltonian of the system is given by $H = \frac{P^2}{2m} + V$

Time dependent Schrödinger wave equation is given by $H\psi = i\hbar \frac{\partial \psi}{\partial t}$

Time independent Schrödinger wave equation is given by $H\psi = E\psi$

where H is Hamiltonian of system.

It is given that total energy E and potential energy of system is V.

3.2 Property of bound state

Bound state

If E > V and there is two classical turning point in which particle is classically trapped then system is called bound state.

Property of Bound state

The energy Eigen value is discrete and in one dimensional system it is non degenerate.

The wave function $\psi_n(x)$ of one dimensional bound state system has *n* nodes if *n* = 0 corresponds to ground state and (n – 1) node if n = 1 corresponds to ground state.

Unbound states

If E > V and either there is one classical turning point or no turning point the energy value is continuous. If there is one turning point the energy eigen value is non-degenerate. If there is no turning point the energy eigen value is degenerate. The particle is said to be unbounded.

If E < V then particle is said to be unbounded and wave function will decay at ± ∞. There is finite probability to find particle in the region.

3.3 Current density

If wave function in one Dimension is $\psi(x)$ then current density is given by

$$J_x = \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$$

which satisfies the continually equation $\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0$

Where $\rho = (\psi^* \psi)$ in general $J = \rho v$ $J = |\psi|^2 v$ where v is velocity of particle?

If J_i, J_r, J_t are incident, reflected and transmitted current density then reflection coefficient R and transmission coefficient T is given by

$$R = \frac{J_r}{J_i} \text{ and } T = \frac{J_t}{J_i}$$

3.4 The free particle in one dimension

$$H\psi = E\psi \quad \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x)$$

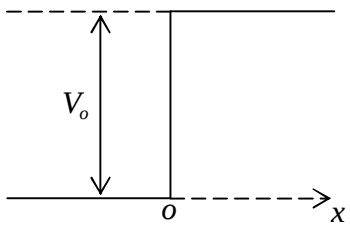
$$\psi(x) = A_+ e^{ikx} + Ae^{-ikx}$$

Energy eigen value $E = \frac{\hbar^2 k^2}{2m}$ where $k = \sqrt{\frac{2mE}{\hbar^2}}$ the eigen values are doubly degenerate

3.5 The Step Potential

The potential step is defined as

$$V(x) = \begin{cases} 0 & x < 0 \\ V_o & x > 0 \end{cases}$$



Case I: E > V_o

$\psi_1 = Ae^{ik_1 x} + Be^{-ik_1 x}$ $\quad x < 0$

$\psi_2 = Ae^{ik_2 x} + Be^{-ik_2 x}$ $\quad x > 0$

Hence, a particle is coming from left so D = 0.

R = reflection coefficient = $\frac{J_{reflected}}{J_{incident}} = R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$

T = transmitted coefficient = $\frac{J_{transmitted}}{J_{incident}} = T = \frac{4k_1k_2}{(k_1+k_2)^2}$

where $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$ $k_2 = \sqrt{\frac{2m(E-V_o)}{\hbar^2}}$

Case II: E < V_o

$\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$ $x < 0$ $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

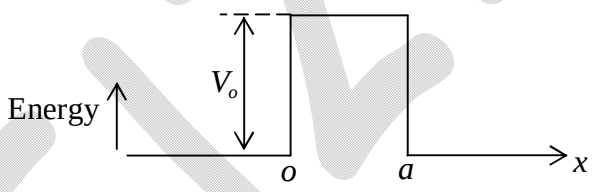
$\psi_{II} = ce^{-k_2x}$ $x > 0$ $k_2 = \sqrt{\frac{2m(V_o-E)}{\hbar^2}}$

$$R = \frac{J_r}{J_t} = 1 \quad \text{and} \quad T = \frac{J_t}{J_i} = 0$$

For case even there is Transmission coefficient is zero there is finite probability to find the particle in $x > 0$.

3.7 Potential Barrier

Potential barrier is shown in figure.



Potential barrier is given by $V(x) = \begin{cases} 0 & x \le 0 \\ V_0 & 0 \le x \le a \\ 0 & x < a \end{cases}$

Case I: $E > V_o$

$\psi_1(x) = \psi_1(x) = Ae^{ik_1x} + Be^{ik_1x}$ $x \le 0$
$\psi_2(x) = \psi_2(x) = Ce^{ik_2x} + De^{ik_2x}$ $0 < x < a$ Where $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$ $k_2 = \sqrt{\frac{2m(E-V_o)}{\hbar^2}}$
$\psi_3(x) = \psi_3(x) = Ee^{ik_1x}$ $x \ge 0$

Transmission coefficient $T = \left[1 + \frac{1}{4 \in (\in -1)} \sin^2\left(\lambda\sqrt{\in -1}\right)\right]^{-1}$

Reflection coefficient $R=\left[1+\frac{4\in(\in-1)}{\sin^2\left(\lambda\sqrt{\in-1}\right)}\right]^{-1}$ Where $\in=\frac{E}{V_o}$, $\lambda=a\sqrt{\frac{2mV_o}{\hbar^2}}$

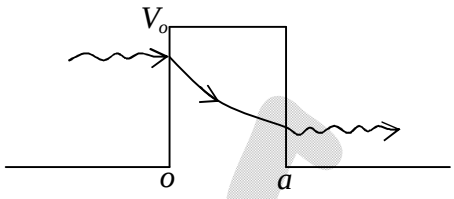
Case II: $E < V_0$

3.7.1 Tunnel Effect

$\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$ $x<0$

$\psi_{II} = Ce^{k_2x} + Be^{-k_2x}$ $0<x<a$

$\psi_{III} = Fe^{ik_1x}$ $x>0$



$R=\frac{1}{4\in(1-\in)}\sin\ h^2\left(\lambda\sqrt{1-\in}\right)$ and $T=1+\frac{1}{4\in(1-\in)}\sin\ h^2\left(\lambda\sqrt{1-\in}\right)$

Where $\lambda=a\sqrt{\frac{2mV_o}{\hbar^2}}$, $\in=\frac{E}{V_o}$

For E << Vo

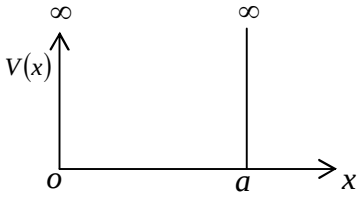
$$T=\frac{16E}{V_o}\left(1-\frac{E}{V_o}\right)e^{-\frac{2a}{\hbar}\sqrt{2m(V_o-E)}}$$

Approximate transmission probability $T\approx e^{-2k_2a}$ where $k_2=\sqrt{\frac{2m(V_o-E)}{\hbar^2}}$

3.8 The Infinite Square Well Potential

The infinite square well potential is defined as as shown in the figure

$$V(x)=\begin{cases}+\infty & x\le 0\\ 0 & 0\le x\le a\\ \infty & x>a\end{cases}$$



Since V(x) is infinite in the region $x<0$ and $x>a$ so the wave function corresponding to the particle will be zero.

The particle is confined only within region $0\le x\le$ a.

Time independent wave Schrödinger wave equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\psi = A\sin kx + B\cos kx$$

B = 0 since wave function must be vanished at boundary ie $x = 0$ so $\psi = A\sin kx$

Energy eigen value for bound state can be find by $ka = n\pi$ where $n = 1, 2, 3...$

The Normalized wave function is for n^{th} state is given by

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$$

Which is energy Eigen value correspondence to n^{th}

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \text{ where n = 1, 2, 3 .....}$$

othonormality relation is given by

$$\int_0^a \sin\frac{m\pi}{L}x\sin\frac{n\pi}{L}x\,dx = \frac{a}{2}\delta_{mn} \quad \text{i.e.}$$

$$= 0 \qquad m \neq n$$

$$= \frac{a}{2} \qquad m = 1$$

If x is position operator P_x P_x is momentum operator and $\psi_n(x)$ is wave function of particle in n^{th} state in one dimensional potential box then $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$ then

$$\langle x\rangle = \int_{-\infty}^{\infty}\psi_n^*(x)x\psi_n(x) = \frac{a}{2}$$

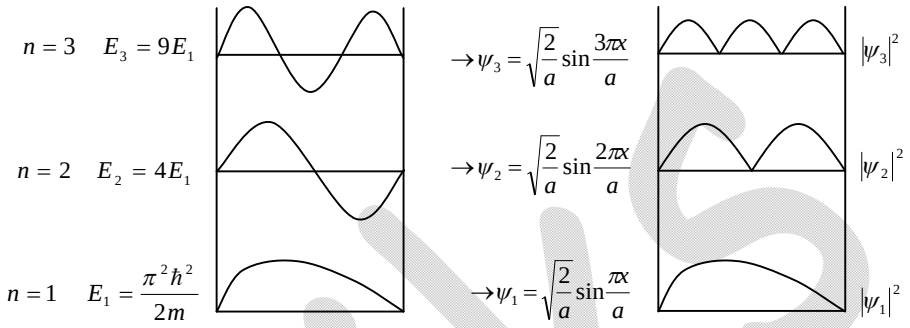
$$\langle x^2\rangle = \int_{-\infty}^{\infty}\psi_n^*(x)x^2\psi_n(x) = \frac{a^2}{2} - \frac{a^2}{2n^2\pi^2}$$

$$\langle P_x\rangle = \int_{-\infty}^{\infty}\psi_n^*(x) - i\hbar\frac{\partial}{\partial x}\psi_n(x) = 0$$

$$\langle P_x^2\rangle = \int_{-\infty}^{\infty}\psi_n^*(x) - \frac{\hbar^2}{2m}\frac{\partial}{\partial x^2}\psi_n(x) = \frac{n^2\pi^2\hbar^2}{a^2}$$

The uncertainty product is given by $\Delta x \Delta P x = n\pi\hbar\sqrt{\frac{1}{12}-\frac{1}{2n^2\pi^2}}$

The wave function and the probability density function of particle of mass m in one dimensional potential box is given by

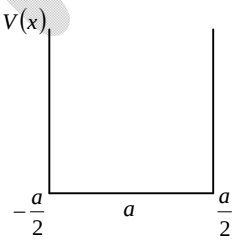


3.8.1 Symmetric Potential

The infinite symmetric well potential is given by

$$V(x)=\infty \qquad x<-\frac{a}{2} \; or \qquad x>\frac{a}{2}$$

$$=0 \qquad -\frac{a}{2}<x<\frac{a}{2}$$



Schrondinger wave function is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi; \qquad -\frac{a}{2}x<\frac{a}{2}$$

$$\psi = A\sin kx + B\cos kx \;\; where \;\; k=\sqrt{\frac{2mE}{\hbar}}$$

$$at \qquad x=\pm\frac{a}{2}, \quad \psi(x)=0$$

$$so \qquad A\sin\frac{ka}{2}+B\cos\frac{ka}{2}=0---(i)$$

$$-A\sin\frac{ka}{2}+B\cos\frac{ka}{2}=0 \qquad ---(ii)$$

Hence parity (π) commute with Hamiltonian (H) then parity must conserve

So wave function have to be either symmetric or anti symmetric

For even parity

$\psi = B\cos kx$ and Bound state energy is given by $\cos\frac{ka}{2} = 0$

$\frac{ka}{2} = 0 \;\; k = \frac{n\pi}{a}$ $\qquad n = 1,3,5,....$

Wave function for even parity is given as $\sqrt{\frac{2}{a}}\cos\frac{n\pi x}{a}$

For odd parity

$\Psi(x)$ = A sin kx and Bound state energy is given by

$\sin\frac{ka}{2} = 0$, $\frac{ka}{2} = 0 \;\; k = \frac{n\pi}{a}$ $\quad n = 2,4,6,.....$

For odd parity Wave function is given as $\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$

The energy eigen value is given by $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ $\quad n = 1,2,3,.....$

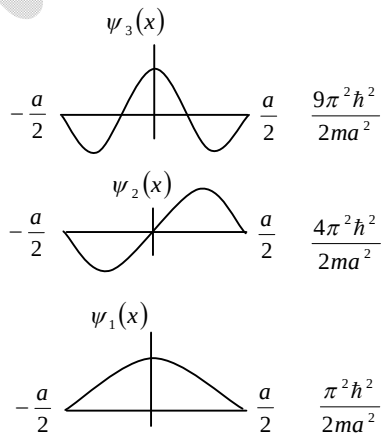
First three wave function is given by

$\psi_1(x) = \sqrt{\frac{2}{a}}\cos\frac{\pi x}{a}$

$\psi_2(x) = \sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}$

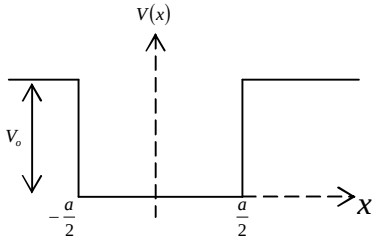
$\psi_3(x) = \sqrt{\frac{2}{a}}\cos\frac{3\pi x}{a}$

where $\sqrt{\frac{2}{a}}$ is normalization constant.



3.9 Finite Square Well Potential

For the Bound state $E < V_o$



Again parity will commute to Hamiltonian

So wave function is either symmetric or

Anti symmetric

For even parity

$$\phi_I(x) = Ae^{\gamma x} \qquad x < -\frac{a}{2}$$

$$\phi_{II}(x) = C\cos kx \qquad -\frac{a}{2} < x < \frac{a}{2}$$

$$\phi_{III}(x) = Ae^{-\gamma x} \qquad x > \frac{a}{2}$$

wave function must be continuous and differentiable at boundaries so using boundary condition at $-\frac{a}{2}$ one will get $\gamma = k\tan\frac{ka}{2}$

$$\eta = \xi\tan\xi \qquad \text{where } \eta = \frac{\gamma a}{2} \quad \xi = \frac{ka}{2}$$

For odd parity

$$\phi_1(x) = Ae^{\gamma x} \qquad x < -\frac{a}{2}$$

$$\phi_2(x) = D\sin kx \qquad -\frac{a}{2} < x < \frac{a}{2}$$

$$\phi_{III}(x) = -Ae^{-\gamma x} \qquad x > \frac{a}{2}$$

using boundary condition one can get

$$\eta = -\xi\cot\xi \quad \text{where } \gamma = \sqrt{\frac{2m(V_o - E)}{\hbar^2}} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

and $n^2 + \xi^2 = \frac{mV_o a^2}{2\hbar^2}$ which is equation of circle.

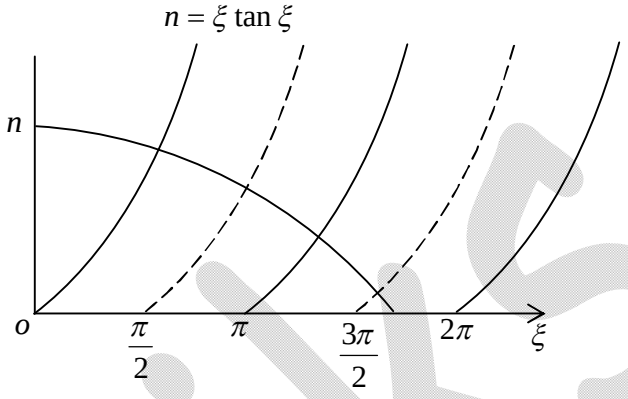
The Bound state energy will be found by solving equation

$n = \xi\tan\xi$ for even

$n = -\xi \cot\xi$ for odd

$$n^2 + \xi^2 = \frac{mV_o a^2}{2\hbar^2}$$

one can solve it by graphical method.

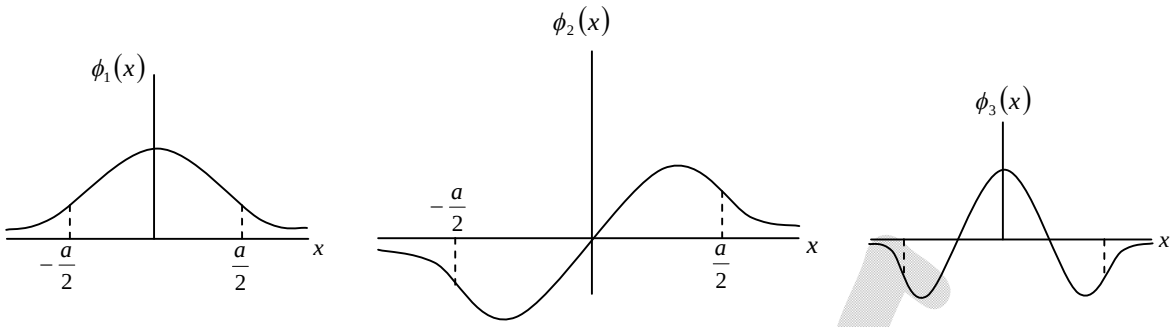


The intersection point of $\eta = \xi\tan\xi$ (solid curve) and $\eta^2 + \xi^2 = \frac{mV_o a^2}{2\hbar^2}$ (circle) give Eigen value for even state and intersection point at $\eta = -\xi\cot\xi$ (dotted curve) and $\eta^2 + \xi^2 = \frac{mV_o a^2}{2\hbar^2}$ (circle) give Eigen value for odd state.

The table below shows the number of bound state for various range of V_0a^2 where V_oa^2 is strength of potential.

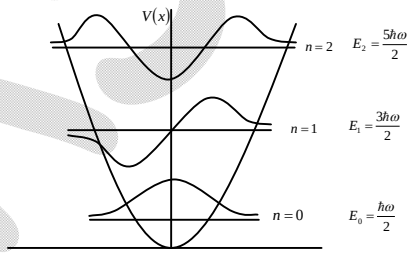
V_oa^2	Even eigen function	Odd eigen function	No. of Bound states
$\frac{\pi^2\hbar^2}{2m}$	1	0	1
$\frac{\pi^2\hbar^2}{2m} < V_0a^2 < \frac{4\pi^2\hbar^2}{2m}$	1	1	2
$\frac{\pi^2\hbar^2}{2m} < V_0a^2 < \frac{9\pi^2\hbar^2}{2m}$	2	1	3
$\frac{9\pi^2\hbar^2}{2m} < V_0a^2 < \frac{16\pi^2\hbar^2}{2m}$	2	2	4

The three bound Eigen function for the square well



3.10 One dimensional Harmonic Oscillator

One dimensional Harmonic oscillator is given by



$$V(x) = \frac{1}{2}m\omega^2 x^2 \qquad -\infty < x < \infty$$

The schrodinger equation is given by

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

It is given that $\varepsilon = \sqrt{\frac{m\omega}{\hbar}}x$ and $k = \frac{2E}{\hbar\omega}$

The wave function of Harmonic oscillator is given by.

$$\phi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(\frac{1}{2^n n!}\right)^{1/2} H_n(\xi)e^{-\frac{\xi^2}{2}}$$

and energy eigen value is given by

$$E_n = (n+1/2)\hbar\omega; \qquad n = 0, 1, 2, 3, ...$$

The wave function of Harmonic oscillator is shown

$H_0(\xi) = 1$, $H_1(\xi) = 2\xi$, $H_2(\xi) = 4\xi^2 - 2$

It ϕ_n and ϕ_m wave function of Harmonic oscillator then $\int_{-\infty}^{\infty}\phi_m(x)\phi_n(x)dx = \delta_{mn}$

Number operator

The Hamiltonian of Harmonic operator is given by $H = \frac{P_x^2}{2m} + \frac{1}{2}m\omega^2 X^2$

Consider dimensioned operator as $\hat{X}, \hat{P}, \hat{H}$ where

$X = \sqrt{\frac{\hbar}{m\omega}}\hat{X} \quad P_x = \sqrt{m\omega\hbar}\hat{P}_x \quad H = \hbar\omega\,\hat{H}$ so $\hat{H} = \frac{1}{2}\left[\hat{P}_x^2 + \hat{X}^2\right]$.

Consider lowering operator $a = \frac{1}{\sqrt{2}}\left[\hat{X} + iP_x\right]$ and raising $a^\dagger = \frac{1}{\sqrt{2}}\left[\hat{X} - iP_x\right]$

$$\hat{H} = \left(N + 1/2\right)$$

where $N = a^\dagger a$ and $H = \left(N + 1/2\right)\hbar\omega$ N is known as number operator

$|n\rangle$ is eigen function of N with eigen value *n*.

$N|n\rangle = n|n\rangle$ and $H|n\rangle = \hbar\omega\left(N + \frac{1}{2}\right)|n\rangle$

$H|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|n\rangle$ where n = 0, 1, 2, 3,……

Commutation of a and $a^\dagger$: $[a, a^\dagger] = 1, [a^\dagger, a] = -1$ and $[N, a] = -a, [N\ a^\dagger] = a^\dagger$

Action of a and $a^\dagger$ operator on $|n\rangle$

$a|n\rangle = \sqrt{n}|n-1\rangle$ *but* $a|0\rangle = 0$

$a^+|n\rangle = \sqrt{n+1}|n+1\rangle$

Expectation value of X, X^2, P_X, P_X^2 in stationary states

$X = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^+\right), \quad P_X = \frac{\left(a - a^+\right)}{\sqrt{2}i}\sqrt{m\omega\hbar}$

$\langle X\rangle = 0, \quad \langle P_X\rangle = 0$

$\langle X^2\rangle = \frac{\hbar}{2m\omega}(2n+1), \quad \langle P_X^2\rangle = \left(n + \frac{1}{2}\right)m\hbar\omega$

$\Delta X\ \Delta P_X = \left(n + \frac{1}{2}\right)\hbar, \quad$ *for* $n = 0;\ \Delta X\ \Delta P_X = \frac{\hbar}{2}$

4. Angular Momentum Problem

Angular momentum in Quantum mechanics is given $L = L_x\hat{i} + L_y\hat{j} + L_z\hat{k}$

Where $L_X = YP_z - ZP_y$; $L_Y = ZP_x - XP_z$; $L_z = XP_y - YP_x$

and $P_X = -i\hbar\frac{\partial}{\partial x}$, $P_Y = -i\hbar\frac{\partial}{\partial y}$, $p_Z = -i\hbar\frac{\partial}{\partial z}$

Commutation relation

$\left[L_x, L_y\right] = i\hbar L_z$, $\left[L_y, L_z\right] = i\hbar L_x$, $\left[L_z, L_x\right] = i\hbar L_y$

$L^2 = L_X^2 + L_Y^2 + L_Z^2$ and $\left[L^2, L_X\right] = 0$, $\left[L^2, L_Y\right] = 0$, $\left[L^2, L_Z\right] = 0$

4.1.1 Eigen Values and Eigen Function

$$L_X = i\hbar\left(Sin\phi\frac{\partial}{\partial\theta} + \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_Y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_Z = -i\hbar\frac{\partial}{\partial\phi}$$

Eigen function of L_Z is $\frac{1}{\sqrt{2\pi}}e^{im\phi}$.

and Eigen value of $L_Z = m\hbar$ where m = 0, ± 1, ± 2...

L^2 operator is given by $L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

Eigen value of L^2 is $l(l+1)\hbar^2$ where l = 0, 1, 2, ...l

Eigen function of L^2 is $P_l^m(\theta)$ where $P_l^m(\theta)$ is **associated Legendre function**

L^2 commute with L_z so both can have common set of Eigen function. $Y_l^m(\theta,\phi) = P_l^m(\theta)e^{im\phi}$ is common set of Eigen function which is known as **spherical harmonics** .

The normalized spherical harmonics are given by

$$Y_l^m(\theta,\phi)=(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)\ !}{(l+m)\ !}}P_l^m(\cos\theta)e^{im\phi} \qquad -l\le m\le l$$

$$Y_0^0(\theta,\phi)=\frac{1}{\sqrt{4\pi}}$$

$$Y_1^1(\theta,\phi)=-\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}\ ,\ Y_1^0(\theta,\phi)=\sqrt{\frac{3}{4\pi}}\cos\theta\ ,\ Y_1^{-1}(\theta,\phi)=\sqrt{\frac{3}{8\pi}}\sin\theta\ \ e^{-i\phi}$$

$L^2Y_l^m(\theta,\phi)=l(l+1)\hbar^2Y_l^m(\theta,\phi)$ $\quad l$ = 0, 1, 2, ……. And

$L_ZY_l^m(\theta,\phi)=m\hbar Y_l^m(\theta,\phi)$ $\quad$ m = -l ,(-l +1) ..0,….. (l – 1)(l) there is $2l+1$

Degeneracy of L^2 is $2l+1$.

Orthogonality Relation $\quad \int_0^{2\pi}d\phi\int_0^{\pi}Y_l^m(\theta,\phi)Y_l^m(\theta,\phi)\sin\theta d\theta=\delta_{ll'}\delta_{mm'}$

4.1.2 Ladder Operator

Let $L_+=L_X+iL_Y$ and $L_-=L_X-iL_Y$

Let us assume $|l,m\rangle$ is ket associated with L^2 and L_Z operator.

$L^2|l,m\rangle=l(l+1)^2|l,m\rangle \quad l=0,1,2,.....$

$L_z|l,,m\rangle=m\hbar|l,m\rangle \qquad m=-l...0,...l$

Action of L_+ and L_- on $|l,m\rangle$ basis

$L_+|l,m\rangle=\sqrt{l(l+1)-m(m+1)}\hbar|l,m+1\rangle$

$L_-|l,m\rangle=\sqrt{l(l+1)-m(m-1)}\hbar|l,m-1\rangle$

Expectation value of L_X and L_Y in direction of $|l,m\rangle$

$\langle L_x\rangle=0\ ,\langle L_y\rangle=0 \quad \langle L_X^2\rangle=\langle L_Y^2\rangle=\frac{\hbar^2}{2}\left[l(l+1)-m^2\right]$

$\Delta L_X\Delta L_Y=\frac{\hbar^2}{2}\left[l(l+1)-m^2\right]$

4.2 Spin Angular Momentum

4.2.1 Stern Gerlach experiment

When silver beam is passed to the inhomogeneous Magnetic field, two sharp trace found on the screen which provides the experimental evidence of spin.

4.2.2 Spin Algebra

$S = S_X \hat{i} + S_Y \hat{j} + S_Z \hat{k}$, $S^2 = S_X^2 + S_Y^2 + S_Z^2$

$\left[S^2, S_X\right] = 0$, $\left[S^2, S_Y\right] = 0$ $\left[S^2, S_Z\right] = 0$ and

$\left[S_X, S_Y\right] = iS_Z$ $\left[S_Y, S_Z\right] = iS_X$ $\left[S_Z, S_X\right] = iS_Y$

$S^2 \left|s, m_s\right\rangle = s(s+1)\hbar^2 \left|s, m_s\right\rangle$ $S_z \left|s, m_s\right\rangle = m\hbar \left|s, m_s\right\rangle$ where $-s \le m_s \le +s$

$S_+ = S_X + iS_Y$ and $S_- = S_X - iS_Y$

$S_+ \left|s, m_s\right\rangle = \hbar\sqrt{s(s+1) - m_s(m_s+1)} \left|s, m_s + 1\right\rangle$

$S_- \left|s, m_s\right\rangle = \hbar\sqrt{s(s+1) - m_s(m_s-1)} \left|s, m_s - 1\right\rangle$

4.2.3 Pauli Spin Matrices

For Spin $\frac{1}{2}$ Pauli matrix $s = \frac{1}{2}, m_s = +\frac{1}{2}, -\frac{1}{2}$

Pauli Matrix is defined as

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

$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$

$\sigma_j \sigma_k + \sigma_k \sigma_j = 0 \qquad (j \neq k)$; Pauli Spin Matrix anticommute.

$$\in_{jkl} = \begin{cases} 1 & \text{if } jkl \text{ is an even permutation of } x, y, z \\ -1 & \text{if } jkl \text{ is an odd permutation of } x, y, z \\ 0 & \text{if any two indices among } j, k, l \text{ are equal} \end{cases}$$

$S_x = \frac{\hbar}{2}\sigma_x, S_y = \frac{\hbar}{2}\sigma_y, S_z = \frac{\hbar}{2}\sigma_z$

$$S_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \quad S_y = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \quad S_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$S_+ = \hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \quad S_- = \hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}$$

$$S^2 = \frac{3\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

For spin ½ the quantum number m takes only two values $m_s = \frac{1}{2}$ and $-\frac{1}{2}$. So that two states are

$$|S, m_s\rangle = \left|\frac{1}{2},\frac{1}{2}\right\rangle \text{and} \left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

$$S^2\left|\frac{1}{2},+\frac{1}{2}\right\rangle = \frac{3\hbar^2}{4}\left|\frac{1}{2},\frac{1}{2}\right\rangle \quad , S^2\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \frac{3\hbar^2}{4}\left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

$$S_z\left|\frac{1}{2},+\frac{1}{2}\right\rangle = \frac{1}{2}\hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle \quad , S_z\left|\frac{1}{2},-\frac{1}{2}\right\rangle = -\frac{1}{2}\hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

$$S_+\left|\frac{1}{2},+\frac{1}{2}\right\rangle = 0 \ , \ S_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle$$

$$S_-\left|\frac{1}{2},\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle \quad , \ S_-\left|\frac{1}{2},-\frac{1}{2}\right\rangle = 0$$

4.3 Total Angular Momentum

Total angular momentum J = L + S , $J = J_x\hat{i} + J_y\hat{j} + J_z\hat{k}$

$|j, m_j\rangle$ is the Eigen ket at J^2 and J_z and $J_+ = J_x + iJ_y \quad J_- = J_x - iJ_y$

$$J^2|j,m_j\rangle = j(j+1)\hbar^2|j,m_j\rangle \ , J_z|j,m_j\rangle = m_j\hbar|j,m_j\rangle$$

$$J_+|j,m_j\rangle = \sqrt{j(j+1)-m_j(m_j+1)}\,|j,m_j-1\rangle$$

$$J_-|j,m_j\rangle = \sqrt{j(j+1)-m_j(m_j-1)}\,|j,m_j-1\rangle$$

$$J = L + S \qquad |l-s| \le j \le |l+s|$$

$$J_z = L_z + S_z \quad -j < m_j < j \quad \text{and} \quad m_l + m_s = m_j$$

5. Two Dimensional Problems in Quantum Mechanics

5.1 Free Particle

$$H\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)=E\psi$$

x and y are independent variable. Thus

$$\psi_n(x,y)=\frac{1}{2\pi}e^{ik_x x}e^{ik_y y}$$

$$=\frac{1}{2\pi}e^{i(\vec{k}\cdot\vec{r})}$$

Energy Eigen value $=\frac{\hbar^2}{2m}\left(k_x^2+k_y^2\right)=\frac{\hbar^2}{2m}k^2$

As total orientation of $\vec{k}$ which preserve its magnitude is infinite. So energy of free particle is infinitely degenerate.

5.2 Square Well Potential

$V(x)=0\le x\le a$ and $0\le y\le a$

∞ otherewise

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)=E\psi$$

The solution of Schrödinger wave equation is given by Wave function

$$\psi_{n_x,n_y}=\sqrt{\frac{4}{a^2}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)$$

Correspondence to energy eigen value

$$E_{nx,ny}=\frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{a^2}+\frac{n_y^2}{a^2}\right)\qquad n_x=1,2,3\ldots \text{ and } n_y=1,2,3\ldots$$

Energy of state	(n_x, n_y)	Degeneracy
Ground state $\frac{2\pi^2\hbar^2}{2ma^2}$	(1, 1)	Non degenerate
First state $\frac{5\pi^2\hbar^2}{2ma^2}$	(1, 2), (2,1)	2
Second state $\frac{8\pi^2\hbar^2}{2ma^2}$	(2, 2)	Non-degenerate

5.3 Harmonic oscillator

Two dimensional isotropic Harmonic oscillators is given by

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + y^2\right)$$

$$E_{n_x n_y} = \left(n_x + n_y + 1\right)\hbar\omega \text{ where } n_x = 0,1,2,3... \; n_y = 0,1,2,3...$$

$$E_n = \left(n+1\right)\hbar\omega$$

degeneracy of the nth state is given by $(n + 1)$ where $n = n_x + n_y$.

6. Three Dimensional Problems in Quantum Mechanics

6.1 Free Particle

$$H\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)=E\psi$$

Hence x, y, z are independent variable. Using separation of variable one can find the

$$\psi_k(x,y,z)=\frac{1}{(2\pi)^{3/2}}e^{ik_n x}e^{ik_y y}e^{ik_z z}=(2\pi)^{-3/2}e^{i\vec{k}.\vec{r}}$$

$$\text{Energy Eigen value}=\frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)=\frac{\hbar^2}{2m}k^2$$

As total orientation of $\vec{k}$ which preserve its magnitude is infinite, the energy of free particle is infinitely degenerate.

6.2 Particle in Rectangular Box

Spinless particle of mass m confined in a rectangular box of sides L_x, L_y, L_z

$V(x,y,z)=0 \le x \le L_x,\ 0 \le y \le L_y,\ 0 \le z \le L_z,$

$= \infty$ other wise .

The Schrodinger wave equation for three dimensional box is given by

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)=E\psi$$

Solution of the Schrödinger is given by Eigen function $\psi_{n_x n_y n_z}$ and energy eigen value is $E_{n_x n_y n_z}$ is given by

$$\psi_{n_x n_y n_z}=\sqrt{\frac{8}{L_x L_y L_z}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right)\sin\left(\frac{n_z\pi z}{L_z}\right)$$

$$E_{n_x n_y n_z}=\frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2}+\frac{n_y^2}{L_y^2}+\frac{n_z^2}{L_z^2}\right)$$

6.2.1 Particle in Cubical Box

For the simple case of cubic box of side a, the

i.e. Lx = Ly = Lz = a

$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{a^3}} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right) \sin\left(\frac{n_z \pi z}{a}\right)$$

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right) \qquad n_x = 1,2,3... \quad n_y = 1,2,3... \quad n_z = 1,2,3...$$

Energy of state	(n_x, n_y, n_z)	Degeneracy
E of ground state $= \frac{3\pi^2\hbar^2}{2ma^2}$	(1, 1, 1)	Non degenerate
E of first excited state $= \frac{6\pi^2\hbar^2}{2ma^2}$	(2, 1, 1) (1, 2, 1) (1, 1, 2	3
E of 2nd excited state $= \frac{9\pi^2\hbar^2}{2ma^2}$	(2, 2, 1) (2, 1, 2) (1, 2, 2)	3

6.3 Harmonic Oscillator

6.3.1 An Anistropic Oscillator

$$V(X,Y,Z) = \frac{1}{2}m\omega_X^2 X^2 + \frac{1}{2}m\omega_Y^2 Y^2 + \frac{1}{2}m\omega_Z^2 Z^2$$

$$E_{n_x n_y n_z} = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z \text{ where}$$

$n_x = 0,1,2,3...$ $n_y = 0,1,2,3...$ $n_x = 0,1,2,3...$

6.3.2 The Isotropic Oscillator

$$\omega_x = \omega_y = \omega_z = \omega$$

$$E_{n_x n_y n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega \text{ where } n = n_x + n_y + n_z \qquad n = 0,1,2,3...$$

Degeneracy is given by $= \frac{1}{2}(n+1)(n+2)$

6.4 Potential in Spherical Coordinate (Central Potential)

Hamiltonion in spherical polar co-ordinate

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

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

L^2 is operator for orbital angular momentum square.

So $Y_l^m(\theta,\phi)$ are the common Eigen state of and L^2 because [H, L^2] = 0 in central force problem and $L^2Y_l^m(\theta,\phi)=l(l+1)\hbar^2Y_l^m(\theta,\phi)$

So $\psi(r,\theta,\phi)$ can be separated as $\psi=f(r)Y_l^m(\theta,\phi)$

$$-\frac{\hbar^2}{2m}\left[\frac{d^2f(r)}{dr^2}+\frac{2}{r}\frac{\partial f}{\partial r}\right]+\frac{l(l+1)\hbar^2}{2mr^2}f(r)+\left(V(r)-E\right)f(r)=0$$

To solve these equations $f(r)=\frac{u(r)}{r}$

So one can get

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[V(r)+\frac{l(l+1)\hbar^2}{2mr^2}-E\right]u=0$$

Where $\frac{l(l+1)\hbar^2}{2mr^2}$ is centrifugal potential and $V(r)+\frac{l(l+1)\hbar^2}{2mr^2}$ is effective potential

The energy Eigen function in case of central potential is written as

$$\psi(r,\theta,\phi)=f(r)Y_l^m(\theta,\phi)=\frac{u(r)}{r}Y_l^m(\theta,\phi)$$

The normalization condition is

$$\int|\psi(r,\theta,\phi)|^2\,d\tau=1$$

$$\int_0^\infty\left|\frac{u(r)}{r}\right|^2r^2dr\int_0^\pi\int_0^{2\pi}\left|Y_l^m(\theta,\phi)^2\right|\sin\theta d\theta d\phi=1$$

$$\int_0^\infty|u(r)|^2\,dr=1 \quad \text{or} \quad \int_0^\infty|R(r)|^2\,r^2dr=1$$

6.4.1 Hydrogen Atom Problem

Hydrogen atom is two body central force problem with central potential is given by

$$V(r) = -\frac{e^2}{4\pi \in_0 r}$$

Time-independent Schrondinger equation on centre of mass reference frame is given by

$$\left[-\frac{\hbar^2}{2m}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(r)\right]\psi(\vec{R},\vec{r}) = E\psi(\vec{R},\vec{r})$$

where $\vec{R}$ is position of c.m and r is distance between proton and electron.

$$\psi(R,\vec{r}) = \phi(\vec{R})\psi(\vec{r})$$

The Schronginger equation is given by

$$\left[-\frac{h^2}{2M}\frac{1}{\phi(\vec{R})}\nabla_R^2\phi(\vec{R})\right] + \left[-\frac{h^2}{2\mu}\frac{1}{\psi(\vec{r})}\nabla_R^2 - \psi(\vec{r}) + V(r)\right] = E$$

Separating R and r part

$$-\frac{\hbar^2}{2M}\nabla^2\phi(\vec{R}) = E_R\phi(\vec{R})$$

$$-\frac{\hbar^2}{2\mu}\nabla_r^2\psi(r) + V(r)\psi(r)$$

Total energy $E = E_R + E_r$

E_R is Energy of centre of mass and E_r is Energy of reduce mass μ

$$\phi(R) = \frac{1}{(2\pi)^{3/2}}e^{i\vec{k}\vec{R}} \qquad E_R = \frac{\hbar^2 k^2}{2M}$$

i.eCentre of mass moves with constant momentum so it is free particle.

Solution of radial part

$$-\frac{h^2}{2\mu}\frac{d^2u(r)}{dr^2} + \left[\frac{l(l+1)h^2}{2\mu r^2} - \frac{e^2}{4\pi \in_0 r}\right]u(r) = E(r)$$

For Hydrogen atom $\mu \approx m_e$

The energy eigen value is given by $E_n = -\frac{m_e e^4}{2(4\pi \in_0)^2 \hbar^2 n^2} = -\frac{13.6}{n^2} eV \quad n = 1, 2, 3...$

And radius of n^{th} orbit is given by $r_n = \frac{4\pi \in_0 \hbar^2 n^2}{m \quad e^2} \quad n = 1, 2, 3...$ where m_e is mass of electron and e is electronic charge.

n is known as participle quantum number which varies as $n = l+1, n+2, ...$ For the given value of n the orbital quantum number n can have value between 0 and $n-1$ (i.e. $l = 0, 1, 2, 3, ... n-1$) and for given value of l the Azimuthal quantum number m varies from $-l$ to l known as magnetic quantum mechanics .

Degeneracy of Hydrogen atom without spin $= n^2$ and if spin is included the degeneracy is given by $g_n = 2\sum_{l=0}^{n-1} 2l+1 = 2n^2$

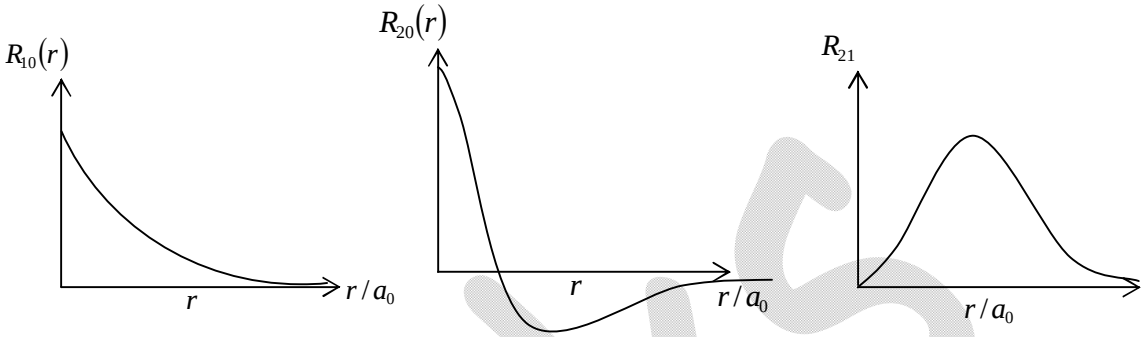
For hydrogen like atom

$E_n = -\frac{13.6z^2}{n^2}$ where z is atomic number of Hydrogen like atom.

Normalized wave function for Hydrogen atom i.e. $R_{nl}(r)$ where n is principle quantum number and l is orbital quantum.

n	l	$E(eV)$	R_{nl}
1	0	$-13.6z^2$	$2\left(\frac{z}{a_0}\right)^{3/2} e^{-zr/a_0}$
2	0	$-3.4\ z^2$	$\left(\frac{z}{2a_0}\right)^{3/2}\left(2-\frac{zr}{a_0}\right) e^{-zr/2a_0}$
2	0	$-3.4\ z^2$	$\frac{1}{\sqrt{24}}\left(\frac{z_0}{a_0}\right)^{3/2}\left(\frac{zr}{a_0}\right) e^{-zr/2a_0}$

The radial wave function for hydrogen atom is Laguerre polynomials and angular part of the wave function is associated Legendre polynomials .



For the n[th] state there is $n-l-1$ node

If R_{nl} is represented by $|n,l\rangle$ then

$$\langle nl|r|nl\rangle = \frac{1}{2}\left[3n^2 - l(l+1)\right]a_0$$

$$\langle nl|r^2|nl\rangle = \frac{1}{2}n^2\left[5n^2 + 1 - 3l(l+1)\right]a_0^2$$

$$\langle nl|r^{-1}|nl\rangle = \frac{1}{n^2 a_0}$$

$$\langle nl|r^{-2}|nl\rangle = \frac{2}{n^3(2l+1)a_0^2}$$

7. Perturbation Theory

7.1 Time Independent Perturbation Theory

7.1.1 Non-degenerate Theory

For approximation methods of stationary states

$$H = H_o + H_P$$

Where H Hamiltonian can be divided into two parts in that H_o can be solved exactly known as unperturbed Hamiltonian and H_p is perturbation in the system **eigen value of H_o is non degenerate**

It is known $H_o|\phi_n\rangle = E_n^o|\phi_n\rangle$ and $\lambda << 1$ $H_p = \lambda W$ where $\lambda << 1$

Now $(H_o + \lambda W)|\psi_n\rangle = E_n|\psi_n\rangle$ where ψ_n is eigen function corresponds to eigen value E_n for the Hamiltonian H

Using Taylor expansion

$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots\ldots$ and $|\psi_n\rangle = |\phi_n\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \ldots\ldots$

First order Energy correction E_n^1 is given by $E_n^{(1)} = \langle\phi_n|W|\phi_n\rangle$

And energy correction up to order in λ is given by $E_n = E_n^1 + \lambda\langle\phi_n|W|\phi_n\rangle$

First order Eigen function correction $|\psi_n^{(1)}\rangle = \sum_{m\neq n}\frac{\langle\phi_m|W|\phi_n\rangle}{E_n^0 - E_m^0}|\phi_m\rangle$

And wave function up to order correction in λ $|\psi_n\rangle = |\phi_n\rangle + \lambda\sum_{m\neq n}\frac{\langle\phi_m|W|\phi_n\rangle}{E_n^0 - E_m^0}|\phi_m\rangle$

Second order energy correction $E_n^{(2)} = \sum_{m\neq n}\frac{|\langle\phi_m|W|\phi_n\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$

Energy correction up to order of λ^2 $E_n = E_0 + \lambda\langle\phi_n|W|\phi_n\rangle + \lambda^2\sum_{m\neq n}\frac{|\langle\phi_m|W|\phi_n\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$

7.1.2 Degenerate Theory

$H|\psi_n\rangle = (H_o + H_p)|\psi_n\rangle = E_n|\psi_n\rangle$

$E_n^{(0)}$ is f fold degenerate $H_o|\phi_{n\alpha}\rangle = E_n^0|\phi_{n\alpha}\rangle \qquad (\alpha = 1,2,3,.....f)$

To determine the Eigen values to first-order and Eigen state to zeroth order for an f-fold degenerate level one can proceed as follows

First for each f-fold degenerate level, determine f x f matrix of the perturbation $\hat{H}_p$

$$\hat{H}_p = \begin{pmatrix} H_{p_{11}} & H_{p_{12}}.....H_{p_{1f}} \\ H_{p_{21}} & H_{p_{22}}.....H_{p_{2f}} \\ . & \\ . & \\ H_{pf_1} & H_{pf_2}.....H_{p_{ff}} \end{pmatrix}$$

where $H_{p_{\alpha\beta}} = \langle\phi_{n\alpha}|H_p|\phi_{n\beta}\rangle$

then diagonalised H_p and find Eigen value and Eigen vector of diagonalized H_p which are $E_{n\alpha}$ and $|\phi_{n\alpha}\rangle$ respectively.

$E_{n\alpha} = E_n^0 + E_{n\alpha}^{(1)}$ and $|\psi_{n\alpha}\rangle = \sum_{\beta=1}^{f} q_{\alpha\beta}|\phi_{n\beta}\rangle$

7.2 Time Dependent Perturbation Theory

The transition probability corresponding to a transition from an initial unperturbed state ψ_i to perturbed $|\psi_f\rangle$ is obtained as

$$P_{if}(t) = -\frac{i}{\hbar}\int_0^1 \langle\psi_f|V(t)|\psi_i\rangle e^{iw_{fi}t'}dt'$$

Where $w_{fi} = \frac{E_f - E_i}{\hbar}$ and $w_{fi} = \frac{\left(\langle\psi_f|H_o|\psi_f\rangle - \langle\psi_i|H_o|\psi_i\rangle\right)}{\hbar}$

8. Variational Method

Variational method is based on energy optimization and parameter variation on the basis of choosing trial wave function.

1. On the basis of physical intuition guess the trial wave function. Say $|\psi_o\rangle = \psi_o(\alpha_1, \alpha_2, \alpha_3, ...\alpha_n)$ where $\alpha_1, \alpha_2, \alpha_3$ are parameter.

2. Find $E_0(\alpha_1, \alpha_2, \alpha_3, ...\alpha_n) = \dfrac{\langle\psi_0(\alpha_1, \alpha_2, \alpha_3, ...\alpha_n)|H|\psi_0(\alpha_1, \alpha_2, \alpha_3, ...\alpha_n)\rangle}{\langle\psi_0(\alpha_1, \alpha_2, \alpha_3, ...\alpha_n)|\psi_0(\alpha_1, \alpha_2, \alpha_3, ...\alpha_n)\rangle}$

3. Find $\dfrac{\partial E_o}{\partial \alpha_i}(\alpha_1, \alpha_2, \alpha_3, ...\alpha_n) = 0$

Find the value of $(\alpha_1, \alpha_2, \alpha_3, ...\alpha)$ so that it minimize E_0.

4. Substitute the value of $(\alpha_1, \alpha_2, \alpha_3, ...\alpha)$ in $E_0(\alpha_1, \alpha_2, \alpha_3, ...\alpha)$ one get minimum value of E_0 for given trial wave function.

5. One can find the upper level of $|\psi_1\rangle$ on the basis that it must be orthogonal to ψ_0 i.e. $\langle\psi_1|\psi_0\rangle = 0$

Once $|\psi_1\rangle$ can be selected the 2, 3, 4 step can be repeated to find energy the first Eigen state.

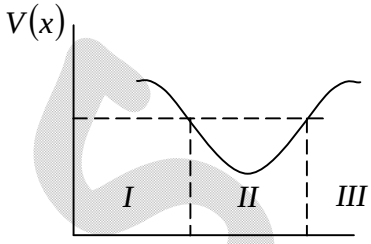
9. The Wentzel-Kramer-Brillouin (WKB) method

WKB method is approximation method popularly derived from semi classical theory

For the case $\left|\frac{d\lambda}{dx}\right| \ll 1$ where $\lambda(x)=\frac{\hbar}{\sqrt{2m(E-V(x))}}$

If potential is given as V(x) then and there is three region

WKB wave function in the first region i.e $x < x_1$



$$\psi_I = \frac{c_1}{\sqrt{P(x)}}\exp\left[-\frac{1}{\hbar}\int_x^{x_1}\left|P(x')\right|dx'\right]$$

WKB wave function in region II: i.e $x_1 < x < x_2$

$$\psi_{II} = \frac{c_2'}{\sqrt{P(x)}}\exp\left[\frac{i}{\hbar}\int P(x')dx\right] + \frac{c_2''}{\sqrt{P(x)}}\exp\left[-\frac{i}{\hbar}\int_x P(x')dx'\right]$$

WKB wave function in region III: i.e $x > x_2$

$$\psi_{III} = \frac{c_3}{\sqrt{P(x)}}\exp\left[-\frac{1}{\hbar}\int_{x_2}^{x}\left|P(x')\right|dx'\right]$$

9.1.1 Quantization of the Energy Level of Bound state

Case I: When both the boundary is smooth

$\oint p(x)dx = (n+\frac{1}{2})\hbar$ where $n = 0,1,2...$

$2\int_{x_1}^{x_2}\sqrt{2m\left(E_n - V(x)\right)}\,dx = \left(n+\frac{1}{2}\right)\hbar$ where $n = 0,\ 1,\ 2,.....$ and x_1 and x_2 are turning point

Case II: When one the boundary is smooth and other is rigid

$$\int_{x_1}^{x_2} p(x)dx = (n+\frac{3}{4})\pi\hbar \quad \text{where } n = 0,1,2...$$

$\int_{x_1}^{x_2}\sqrt{2m\left(E_n - V(x)\right)}\,dx = \left(n+\frac{3}{4}\right)\pi\hbar$ where $n = 0,\ 1,\ 2,.....$ and x_1 and x_2 are turning points

Case III: When both boundary of potential is rigid

$\int_{x_1}^{x_2} p(x)dx = (n+1)\pi\hbar$ where $n = 0,1,2...$

$\int_{x_1}^{x_2} \sqrt{2m\left(E_n - V(x)\right)}\ dx = (n+1)\pi\hbar$ where $n = 0,\ 1,\ 2,.....$ and x_1 and x_2 are turning points .

9.1.2 Transmission probability from WKB

T is defined as transmission probability through potential barrier V is given by

$T = \exp -2\gamma$ where $\gamma = \frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m\left(E_n - V(x)\right)}\ dx$ and x_1 and x_2 are turning points.

10. Identical Particles

Identical particle in classical mechanics are distinguishable but identical particle in quantum mechanics are Indistinguishable.

Total wave function of particles are either totally symmetric or totally anti-symmetric.

11.1 Exchange Operator

Exchange operator P_{ij} as an operator as that when acting on an N-particle wave function $\psi(\xi_1\xi_2\xi_3....\xi_i...\xi_j...\xi_N)$ interchanges i and j.

i.e $P_{ij}\psi(\xi_1\xi_2\xi_3....\xi_i...\xi_j...\xi_N) = \pm\psi(\xi_1\xi_2\xi_3....\xi_j...\xi_i...\xi_N)$

$+$ sign is for symmetric wave function ψ_s and $-$ sign for anti symmetric wave function ψ_a.

11.2 Particle with Integral Spins

Particle with integral spins or boson has symmetric states.

$$\psi_s(\xi_1\xi_2) = \frac{1}{\sqrt{2}}\left[\psi(\xi_1,\ \xi_2)+\psi(\xi_2,\ \xi_1)\right]$$

For three identical particle:

$$\psi_s(\xi_1\,\xi_2\,\xi_3) = \frac{1}{\sqrt{6}}\begin{bmatrix}\psi(\xi_1,\xi_2,\xi_3)+\psi(\xi_1,\xi_3,\xi_2)+\psi(\xi_2,\xi_3,\xi_1)\\ +\psi(\xi_2,\xi_1,\xi_3)+\psi(\xi_3,\xi_1,\xi_2)+\psi(\xi_3,\xi_2,\xi_1)\end{bmatrix}$$

For boson total wave function(space and spin) is symmetric i.e if space part is symmetric spin part will also symmetric and if space part is ant symmetric space part will also also anti symmetric.

11.3 Particle with Half-integral Spins

Particle with half-odd-integral spins or fermions have anti-symmetric.

For two identical particle**:**

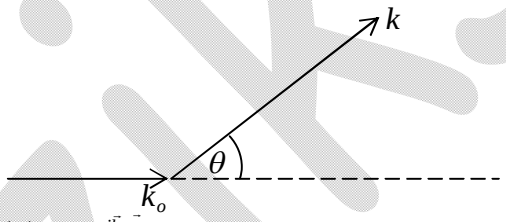
$$\psi_a(\xi_1\xi_2) = \frac{1}{\sqrt{2}}\left[\psi(\xi_1,\xi_2)-\psi(\xi_2,\xi_1)\right]$$

For three identical particle**:**

$$\psi_a(\xi_1\ \ \xi_2\ \ \xi_3)=\frac{1}{\sqrt{6}}\begin{bmatrix}\psi(\xi_1,\ \xi_2,\ \xi_3)-\psi(\xi_1,\ \xi_3,\ \xi_2)+\psi(\xi_2,\ \xi_3,\ \xi_1)\\-\psi(\xi_2,\ \xi_1,\ \xi_3)+\psi(\xi_3,\ \xi_1,\ \xi_2)-\psi(\xi_3,\ \xi_2,\ \xi_1)\end{bmatrix}$$

For fermions total wave function(space and spin) is anti symmetric .ie if space part is symmetric spin part will anti symmetric and if space part is ant symmetric space part will also symmetric.

11. Scattering in Quantum Mechanics



Incident wave is given by $\phi_{inc}(r)=Ae^{i\vec{k}_o.\vec{r}}$. If particle is scattered with angle θ which is angle between incident and scattered wave vector $\vec{k}_o$ and $\vec{k}$ Scattered wave is given by $\phi_{sc}(r)=Af(\theta,\phi)\frac{e^{i\vec{k}.\vec{r}}}{r}$, where $f(\theta,\phi)$ is called scattering amplitude wave function.

ψ is superposition of incident and scattered wave $\psi\approx A\left[e^{ik_or}+f(\theta,\phi)\frac{e^{ik_or}}{r}\right]$

differential scattering cross section is given by $\frac{d\sigma}{d\Omega}=\frac{k}{k_o}|f(\theta,\phi)|^2$ where Ω is solid angle

For elastic collision $\frac{d\sigma}{d\Omega}=|f(\theta,\phi)|^2$

If potential is given by V and reduce mass of system is μ then

$$\frac{d\sigma}{d\Omega}=|f(\theta,\phi)|^2=\frac{\mu^2}{4\pi\hbar^2}\left|\int e^{-ikr'}V(r')\psi(r')d^3r'\right|^2$$

11.1 Born Approximation

Born approximation is valid for weak potential V(r)

$$f(\theta,\phi) = -\frac{2\mu}{\hbar^2 q}\int_0^\infty r'V(r')\sin(qr')\,dr'$$

Where $q = \left|\vec{k_o} - \vec{k}\right| = 2k\sin\frac{\theta}{2}$ for and for $\left|\vec{k_o}\right| = \left|\vec{k}\right|$ $\frac{d\sigma}{d\Omega} = \frac{4\mu^2}{\hbar^4 q^2}\left|\int_0^\infty r'V(r')\sin(qr')\,dr'\right|^2$

11.2 Partial Wave Analysis

Partial wave analysis for elastic scattering

For spherically symmetric potential one can assume that the incident plane wave is in z-direction hence $\phi_{inc}(r) = \exp(ikr\cos\theta)$. So it can be expressed in term of a superposition of angular momentum Eigen state, each with definite angular momentum number l

$e^{ik\cdot r} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+l) J_l(kr) p_l(\cos\theta)$, where J_l is Bessel's polynomial function and P_l is Legendre polynomial.

$$\psi(r,\theta) = \sum_{l=0}^{\infty} i^l (2l+1) J_l(kr) P_l(\cos\theta) + f(\theta)\frac{e^{ikr}}{r}$$

$$f(\theta) = \frac{1}{k}\sum(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta)$$

Total cross section is given by

$$\sigma = \sum_{l=0}^{\infty}\sigma_l = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

Where σ_l is called the partial cross section corresponding to the scattering of particles in various angular momentum states and δ_l is phase shift .

12. Relativistic Quantum Mechanics

12.1 Klein Gordon equation

The non-relativistic equation for the energy of a free particle is

$\frac{p^2}{2m} = E$ and $\Rightarrow \frac{p^2}{2m}\psi = E\psi$ $\Rightarrow \frac{p^2}{2m}\psi = i\hbar\frac{\partial\psi}{\partial t}$ where

$p = -i\hbar\nabla$ is the momentum operator (∇ being the del operator).

The Schrödinger equation suffers from not being relativistic ally covariant, meaning it does not take into account Einstein's special relativity .It is natural to try to use the identity from special relativity describing the energy: $\sqrt{p^2c^2 + m^2c^4} = E$ Then, just inserting the quantum mechanical operators for momentum and energy yields the equation $\sqrt{-\hbar^2c^2\nabla^2 + m^2c^4}\psi = i\hbar\frac{\partial\psi}{\partial t}$

This, however, is a cumbersome expression to work with because the differential operator cannot be evaluated while under the square root sign.

which simplifies to $-\hbar^2c^2\nabla^2\psi + m^2c^4 = -\frac{\partial^2\psi}{\partial t^2}$

Rearranging terms yields $\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi + \frac{m^2c^2\psi}{\hbar^2} = E\psi$

Since all reference to imaginary numbers has been eliminated from this equation, it can be applied to fields that are real valued as well as those that have complex values.

Using the inverse of the Murkowski metric we ge $-\eta^{\mu\nu}\partial_{\mu\nu}\psi + \frac{m^2c^2}{\hbar^2}\psi = 0$ where

$(\Box + \mu^2)\psi = 0$

In covariant notation. This is often abbreviated as $(\Box+\mu^2)\psi=0$ where $\mu=\frac{mc}{\hbar}$ and

$\Box=\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\nabla^2$

This operator is called the d'Alembert operator . Today this form is interpreted as the relativistic field for a scalar (i.e. spin -0) particle. Furthermore, any solution to the Dirac equation (for a spin-one-half particle) is automatically a solution to the Klein–Gordon equation, though not all solutions of the Klein–Gordon equation are solutions of the Dirac equation.

The Klein–Gordon equation for a free particle and dispersion relation

Klein –Gordon relation for free particle is given by $\nabla^2\psi-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}=E\psi$

with the same solution as in the non-relativistic case:

dispersion relation from free wave equation $\psi(r,t)=\exp i(k.r-\omega t)$ which can be obtained by putting the value of ψ in $\nabla^2\psi-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}=E\psi$ equation we will get dispersion relation which is given by $-k^2+\frac{\omega^2}{k^2}=\frac{m^2c^2}{\hbar^2}$.

12.2 Dirac Equation

searches for an alternative *relativistic* equation starting from the generic form describing evolution of wave function:

$$i\frac{\partial}{\partial t}=\hat{H}\Psi$$

If one keeps first order derivative of time, then to preserve Lorentz invariance, the space coordinate derivatives must be of the first order as well. Having all energy-related operators (E, p, m) of the same first order:

$$\hat{E}=i\frac{\partial}{\partial t} \text{ and } \hat{p}_x=-i\frac{\partial}{\partial x},\hat{p}_y=-i\frac{\partial}{\partial y},\hat{p}_z=-i\frac{\partial}{\partial z}$$

$$\hat{E}\Psi = \left(\alpha_1 \hat{p}_x + \alpha_2 \hat{p}_y + \alpha_3 \hat{p}_z + \beta m\right)\Psi$$

By acting with left-and right-hand operators twice, we get

$$\hat{E}^2\Psi = \left(\alpha_1 \hat{p}_x + \alpha_2 \hat{p}_y + \alpha_3 \hat{p}_z + \beta m\right)\left(\alpha_1 \hat{p}_x + \alpha_2 \hat{p}_y + \alpha_3 \hat{p}_z + \beta m\right)\Psi$$

which must be compatible with the Klein-Gordon equation

$$\hat{E}^2\Psi = \left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2 + m^2\right)\Psi$$

This implies that

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 0, \text{ for } i \neq j$$

$$\alpha_i \beta + \beta \alpha_i = 0$$

$$\alpha_i^2 = 1$$

$$\beta^2 = 1$$

Therefore, parameters α and β cannot be numbers. However, it may and does work if they are matrices, the lowest order being 4×4. Therefore, ψ must be 4-component vectors. Popular representations are

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where σ_i are 2×2 Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The equation is usually written using γμ-matrices, where $\gamma_i = \beta\alpha_i$ for

The equation is usually written using γμ-matrices, where $\gamma_i = \beta\alpha_i$ for $i = 1,2,3$ and $\gamma_0 = \beta$ (just multiply the above equation with matrix β and move all terms on one side of the equation):

$$\left(i\gamma_\mu \frac{\partial}{\partial x_\mu} - m\right)\Psi = 0 \text{ where } \gamma_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \text{ and } \gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Find solution for particles at rest, i.e. p=0:

$$\left(i\gamma_0\frac{\partial}{\partial t}-m\right)\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix}=0$$

$$i\frac{\partial}{\partial t}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\Psi_A\\ \Psi_B\end{pmatrix}=m\begin{pmatrix}\Psi_A\\ \Psi_B\end{pmatrix}$$

It has two positive energy solutions that correspond to two spin states of spin-½ electrons:

$$\Psi_A=e^{-imt}\begin{pmatrix}1\\ 0\end{pmatrix}\text{ and }\Psi_A=e^{-imt}\begin{pmatrix}0\\ 1\end{pmatrix}$$

and two symmetrical negative-energy solutions

$$\Psi_B=e^{+imt}\begin{pmatrix}1\\ 0\end{pmatrix}\text{ and }\Psi_B=e^{+imt}\begin{pmatrix}0\\ 1\end{pmatrix}$$