Lectures
IN
Quantum Mechanics-III
For
Fourth Year Students
Faculties of Science and Education

Prepared By

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Chapter (1)
Different Coordinate Systems

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Different Coordinate Systems

1. Introduction

Coordinate systems is an artificial mathematical tool that used to describe the position of an object in space.. There are three coordinate systems:

1. One dimension coordinate system (1D).
2. Two dimension coordinate system (2D).
3. Three dimension coordinate system (3D).

In physics basic laws are first introduced for a point partile and then laws are extended to system of particles or continuous bodies. Therefore, we also begin the discussion with point particle and later on we will study collection of particles or rigid body.

To write equations governing the dynamics of a aprticle we need its position vectors, velocity, acceleration etc. Therefore we first introduce these elementaty concepts.

1-1: (1D) Coordinate system

The easiest coordinate system use to describe the location of objects in one dimensional space. For example, to describe the location of a train along a straight section of track that runs in the East-West direction. {Figure (1)}.

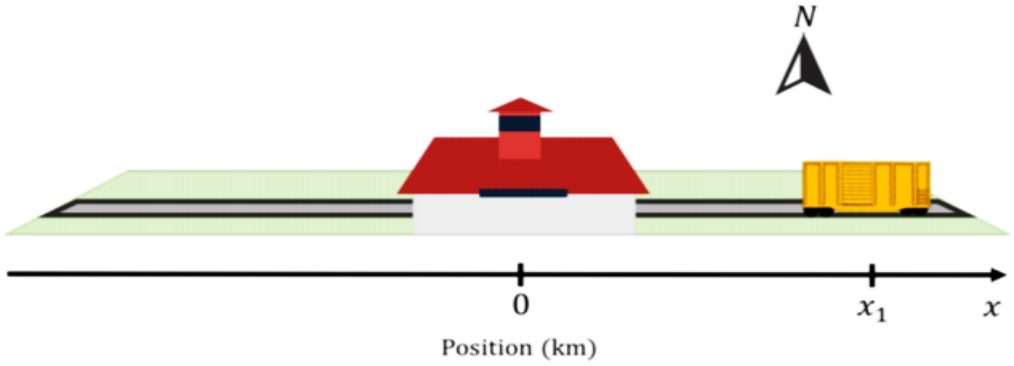


Figure (1): A 1D coordinate system describing the position of a train.

** In order to fully specify a one-dimensional coordinate system we need to choose:

1- The location of the origin.

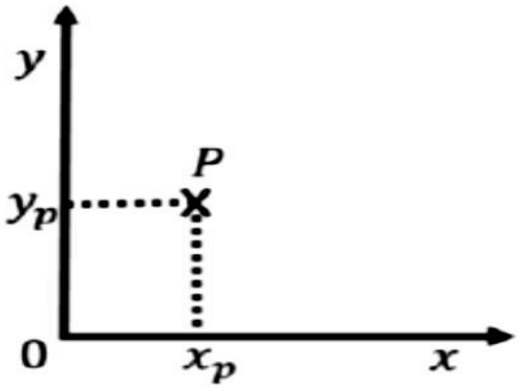
2- The direction in which the coordinate, x, increases.

3- The units in which we wish to express x.

In one dimension, it is common to use the variable x to define the position along the "x-axis". The x-axis is our coordinate system in one dimension.

1-2 : 2D Coordinate systems

To describe the position of an object in two dimensions, we need to specify two numbers. The easiest way to do this is to define two axes, x and y. Figure (2) shows an example of such a coordinate system. The axes are perpendicular in "Cartesian" coordinate system.



Figure(2): Example of Cartesian coordinate system and a point P with coordinates (xp, yp).

Another common choice is a "polar" coordinate system, where the position of an object is specified by a distance to the origin, r, and an angle, relative to a specified direction, as shown in Figure (3). Often, a polar coordinate system is defined alongside a Cartesian system, so that r is the distance to the origin of the Cartesian system and is the angle with respect to the axis.

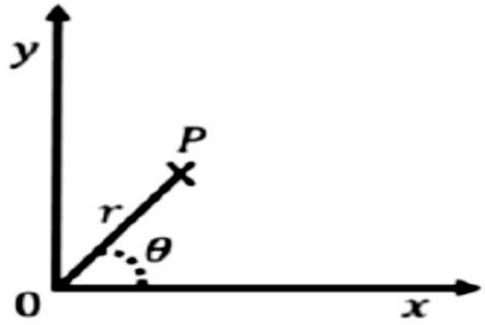


Figure (3): Example of a polar coordinate system and a point P with coordinates (r,ɵ) .

One can easily convert between the two Cartesian coordinates, x and y, and the two corresponding polar coordinates, r and ɵ:

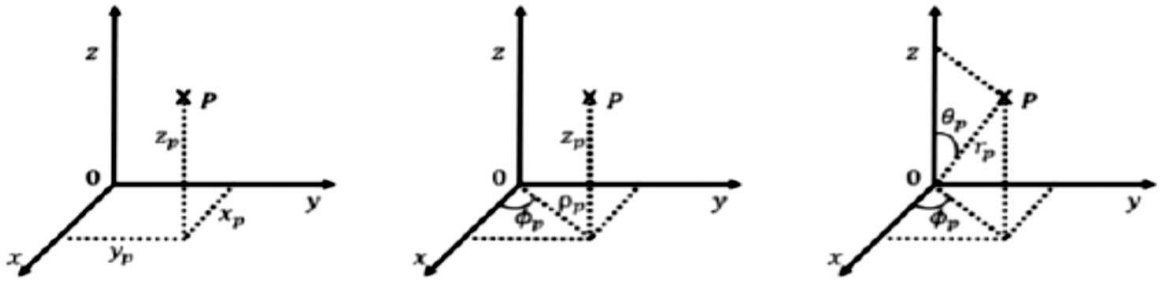
$$x = r\cos(\theta)$$
$$y = r\sin(\theta)$$
$$r = \sqrt{x^2 + y^2}$$
$$\tan(\theta) = \frac{y}{x}$$

Polar coordinates are often used to describe the motion of an object moving around a circle, as this means that only one of the coordinates (□) changes with time.

1-3 : 3D Coordinate systems

In three dimensions, we need to specify three numbers to describe the position of an object. In a three dimensional Cartesian coordinate system, we simply add a third axis, z, that is mutually perpendicular to both x and y. The position of an object can then be specified by using the three coordinates x, y, and z. **Two additional coordinate systems are common in three dimensions: "cylindrical" and "spherical" coordinates.** All three systems are illustrated in Figure (4) superimposed onto the Cartesian system.

Figure (4): Cartesian (left), cylindrical (center) and spherical (right) coordinate systems used in three dimensions.



Cylindrical coordinates can be thought of as an extension of the polar coordinates. We keep the same Cartesian coordinate z to indicate the height above the x-y plane, however, we use the azimuthal angle, θ , and the radius, r , to describe the position of the projection of a point onto the x-y plane. Φ is the angle between the x axis and the line from the origin to the projection of the point in the x-y plane and ρ is the distance between the point and the z axis.

**The cylindrical coordinates are related to the Cartesian coordinates by:

$$\rho = \sqrt{x^2 + y^2}$$
$$\tan(\phi) = \frac{y}{x}$$
$$z = z$$

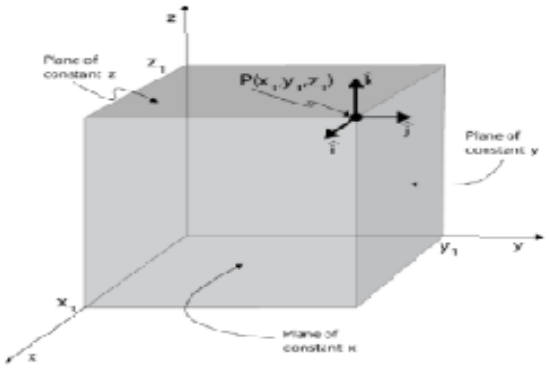
In spherical coordinates, a point P is described by the radius, r, the polar angle θ , and the azimuthal angle Φ. The radius is the distance between the point and the origin. The polar angle is the angle with the z axis that is made by the line from the origin to the point. The azimuthal angle is defined in the same way as in polar coordinates.

**The spherical coordinates are related to the Cartesian coordinates by:

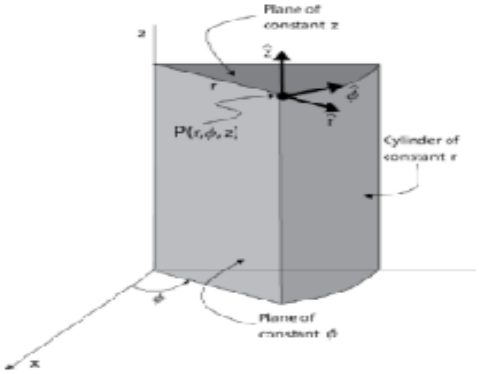
$$r = \sqrt{x^2 + y^2 + z^2}$$
$$\cos(\theta) = \frac{z}{r} = \frac{z}{\sqrt{x^2 + y^2 + z^2}}$$
$$\tan(\phi) = \frac{y}{x}$$

Unit Vectors in Rectangular , Cylindrical and Spherical Coordinates

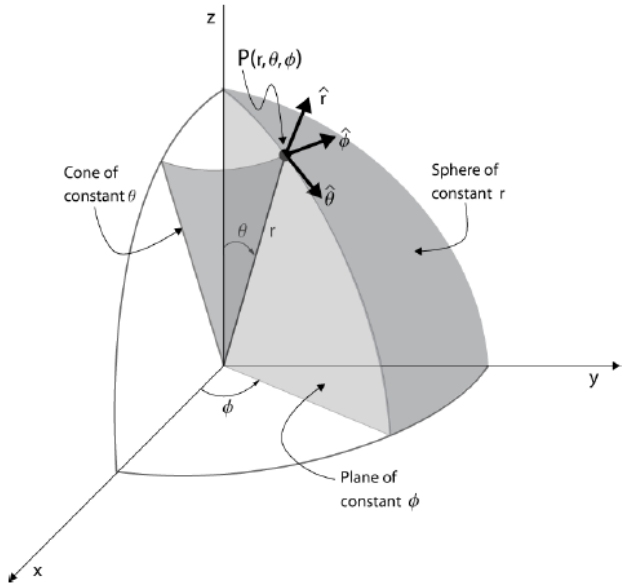
In *rectangular coordinates* a point P is specified by x, y, and z, where these values are all measured from the origin (see figure at right). A vector at the point P is specified in terms of three mutually perpendicular components with unit vectors $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$, and $\hat{\mathbf{k}}$ (also called $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$). The unit vectors $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$, and $\hat{\mathbf{k}}$ form a right-handed set; that is, if you push $\hat{\mathbf{i}}$ into $\hat{\mathbf{j}}$ with your right hand, your right thumb will point along $\hat{\mathbf{k}}$ direction.



In *cylindrical coordinates* a point P is specified by r, ϕ, z, where ϕ is measured from the x axis (or x-z plane) (see figure at right). A vector at the point P is specified in terms of three mutually perpendicular components with unit vectors $\hat{\mathbf{r}}$ perpendicular to the cylinder of radius r, $\hat{\boldsymbol{\varphi}}$ perpendicular to the plane through the z axis at angle ϕ, and $\hat{\mathbf{z}}$ perpendicular to the x-y plane at distance z. The unit vectors $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\varphi}}$, $\hat{\mathbf{z}}$ form a right-handed set.



In *spherical coordinates* a point P is specified by r, θ, ϕ, where r is measured from the origin, θ is measured from the z axis, and ϕ is measured from the x axis (or x-z plane) (see figure at right). With z axis up, θ is sometimes called the *zenith* angle and ϕ the *azimuth* angle. A vector at the point P is specified in terms of three mutually perpendicular components with unit vectors $\hat{\mathbf{r}}$ perpendicular to the sphere of radius r, $\hat{\boldsymbol{\theta}}$ perpendicular to the cone of angle θ, and $\hat{\boldsymbol{\varphi}}$ perpendicular to the plane through the z axis at angle ϕ. The unit vectors $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$, $\hat{\boldsymbol{\varphi}}$ form a right-handed set.



Infinitesimal lengths and volumes

An infinitesimal length in the *rectangular* system is given by

$$d\boldsymbol{L} = \sqrt{dx^2 + dy^2 + dz^2} \tag{1}$$

and an infinitesimal volume by

$$dv = dx\,dy\,dz \tag{2}$$

In the *cylindrical* system the corresponding quantities are

$$d\boldsymbol{L} = \sqrt{dr^2 + r^2 d\phi^2 + dz^2} \tag{3}$$

and

$$dv = dr\; r\,d\phi\; dz \tag{4}$$

In the *spherical* system we have

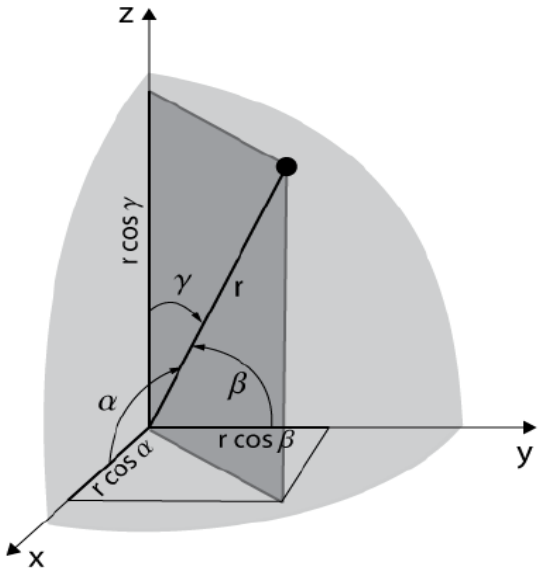
$$d\boldsymbol{L} = \sqrt{dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta\; d\phi^2} \tag{5}$$

and

$$dv = dr\, r\, d\theta\; r\, \sin\theta\, d\phi \tag{6}$$

Direction cosines and coordinate-system transformation

As shown in the figure on the right, the projection x of the scalar distance r on the x axis is given by $r\cos\alpha$ where α is the angle between r and the x axis. The projection of r on the y axis is given by $r\cos\beta$, and the projection on the z axis by $r\cos\gamma$. Note that $\gamma=\theta$ so $\cos\gamma=\cos\theta$.



The quantities $\cos\alpha$, $\cos\beta$, and $\cos\gamma$ are called the *direction cosines*. From the theorem of Pythagoras,

$$\cos^2\alpha+\cos^2\beta+\cos^2\gamma=1 \qquad (7)$$

The scalar distance r of a spherical coordinate system transforms into rectangular coordinate distance

$$x=r\cos\alpha=r\sin\theta\cos\phi \qquad (8)$$
$$y=r\cos\beta=r\sin\theta\sin\phi \qquad (9)$$
$$z=r\cos\gamma=r\cos\theta \qquad (10)$$

from which

$$\left.\begin{aligned}\cos\alpha&=\sin\theta\cos\phi \qquad (11)\\ \cos\beta&=\sin\theta\sin\phi \qquad (12)\\ \cos\gamma&=\cos\theta \qquad (13)\end{aligned}\right\}\text{direction cosines}$$

As the converse of (8), (9), and (10), the spherical coordinate values (r,θ,ϕ) may be expressed in terms of rectangular coordinate distances as follows:

$$r=\sqrt{x^2+y^2+z^2} \qquad r\geq 0 \qquad (14)$$

$$\theta=\cos^{-1}\frac{z}{\sqrt{x^2+y^2+z^2}} \qquad (0\leq\theta\leq\pi) \qquad (15)$$

$$\phi=\tan^{-1}\frac{y}{x} \qquad (16)$$

From these and similar coordinate transformations of spherical to rectangular and rectangular to spherical coordinates, we may express a vector **A** at some point P with spherical components A_r, A_θ, A_ϕ as the rectangular components A_x, A_y, and A_z, where

$$A_x = A_r \sin\theta \cos\phi + A_\theta \cos\theta \cos\phi - A_\phi \sin\phi \qquad (17)$$
$$A_y = A_r \sin\theta \sin\phi + A_\theta \cos\theta \sin\phi + A_\phi \cos\phi \qquad (18)$$
$$A_z = A_r \cos\theta - A_\theta \sin\theta \qquad (19)$$

Note that the direction cosines are simply the dot products of the spherical unit vector $\hat{\mathbf{r}}$ with the rectangular unit vectors $\hat{\mathrm{x}}$, $\hat{\mathrm{y}}$, and $\hat{\mathrm{z}}$:

$$\hat{\mathbf{r}} \cdot \hat{\mathbf{x}} = \sin\theta\cos\phi = \cos\alpha \qquad (20)$$
$$\hat{\mathbf{r}} \cdot \hat{\mathbf{y}} = \sin\theta\sin\phi = \cos\beta \qquad (21)$$
$$\hat{\mathbf{r}} \cdot \hat{\mathbf{z}} = \cos\theta = \cos\gamma \qquad (22)$$

These and other dot product combinations are listed in the following table:

		Rectangular			*Cylindrical*			*Spherical*		
		$\hat{\mathbf{x}}$	$\hat{\mathbf{y}}$	$\hat{\mathbf{z}}$	$\hat{\mathbf{r}}$	$\hat{\boldsymbol{\varphi}}$	$\hat{\mathbf{z}}$	$\hat{\mathbf{r}}$	$\hat{\boldsymbol{\theta}}$	$\hat{\boldsymbol{\varphi}}$
Rectangular	$\hat{\mathbf{x}}$	1	0	0	$\cos\phi$	$-\sin\phi$	0	$\sin\theta\cos\phi$	$\cos\theta\cos\phi$	$-\sin\phi$
	$\hat{\mathbf{y}}$	0	1	0	$\sin\phi$	$\cos\phi$	0	$\sin\theta\sin\phi$	$\cos\theta\sin\phi$	$\cos\phi$
	$\hat{\mathbf{z}}$	0	0	1	0	0	1	$\cos\theta$	$-\sin\theta$	0
Cylindrical	$\hat{\mathbf{r}}$	$\cos\phi$	$\sin\phi$	0	1	0	0	$\sin\theta$	$\cos\theta$	0
	$\hat{\boldsymbol{\varphi}}$	$-\sin\phi$	$\cos\phi$	0	0	1	0	0	0	1
	$\hat{\mathbf{z}}$	0	0	1	0	0	1	$\cos\theta$	$-\sin\theta$	0
Spherical	$\hat{\mathbf{r}}$	$\sin\theta\cos\phi$	$\sin\theta\sin\phi$	$\cos\theta$	$\sin\theta$	0	$\cos\theta$	1	0	0
	$\hat{\boldsymbol{\theta}}$	$\cos\theta\cos\phi$	$\cos\theta\sin\phi$	$-\sin\theta$	$\cos\theta$	0	$-\sin\theta$	0	1	0
	$\hat{\boldsymbol{\varphi}}$	$-\sin\phi$	$\cos\phi$	0	0	1	0	0	0	1

Note that the unit vectors $\hat{\mathbf{r}}$ in the cylindrical and spherical systems are *not* the same. For example,

Spherical	*Cylindrical*
$\hat{\mathbf{r}} \cdot \hat{\mathbf{x}} = \sin\theta\cos\phi$	$\hat{\mathbf{r}} \cdot \hat{\mathbf{x}} = \cos\phi$
$\hat{\mathbf{r}} \cdot \hat{\mathbf{y}} = \sin\theta\sin\phi$	$\hat{\mathbf{r}} \cdot \hat{\mathbf{y}} = \sin\phi$
$\hat{\mathbf{r}} \cdot \hat{\mathbf{z}} = \cos\theta$	$\hat{\mathbf{r}} \cdot \hat{\mathbf{z}} = 0$

The fundamental parameters of the rectangular, cylindrical, and spherical coordinate systems are summarized in the following table:

Coordinate system	Coordinates	Range	Unit vectors	Length elements	Coordinate surfaces	
Rectangular	x	$-\infty$ to $+\infty$	$\hat{\mathbf{x}}$ or $\hat{\mathbf{i}}$	dx	Plane	x=constant
	y	$-\infty$ to $+\infty$	$\hat{\mathbf{y}}$ or $\hat{\mathbf{j}}$	dy	Plane	y=constant
	z	$-\infty$ to $+\infty$	$\hat{\mathbf{z}}$ or $\hat{\mathbf{k}}$	dz	Plane	z=constant
Cylindrical	r	0 to ∞	$\hat{\mathbf{r}}$	dr	Cylinder	r=constant
	ϕ	0 to 2π	$\hat{\boldsymbol{\varphi}}$	$r\,d\phi$	Plane	ϕ=constant
	z	$-\infty$ to $+\infty$	$\hat{\mathbf{z}}$	dz	Plane	z=constant
Spherical	r	0 to ∞	$\hat{\mathbf{r}}$	dr	Sphere	r=constant
	θ	0 to π	$\hat{\boldsymbol{\theta}}$	$r\,d\theta$	Cone	θ=constant
	ϕ	0 to 2π	$\hat{\boldsymbol{\varphi}}$	$r\sin\theta\,d\phi$	Plane	ϕ=constant

The following two tables give the unit vector dot products in rectangular coordinates for both rectangular-cylindrical and rectangular-spherical coordinates.

	$\hat{\mathbf{x}}$	$\hat{\mathbf{y}}$	$\hat{\mathbf{z}}$
$\hat{\mathbf{r}}$	$\dfrac{x}{\sqrt{x^2+y^2}}$	$\dfrac{y}{\sqrt{x^2+y^2}}$	0
$\hat{\boldsymbol{\varphi}}$	$\dfrac{-y}{\sqrt{x^2+y^2}}$	$\dfrac{x}{\sqrt{x^2+y^2}}$	0
$\hat{\mathbf{z}}$	0	0	1

	$\hat{\mathbf{x}}$	$\hat{\mathbf{y}}$	$\hat{\mathbf{z}}$
$\hat{\mathbf{r}}$	$\dfrac{x}{\sqrt{x^2+y^2+z^2}}$	$\dfrac{y}{\sqrt{x^2+y^2+z^2}}$	$\dfrac{z}{\sqrt{x^2+y^2+z^2}}$
$\hat{\boldsymbol{\theta}}$	$\dfrac{xz}{\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}}$	$\dfrac{yz}{\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}}$	$-\dfrac{\sqrt{x^2+y^2}}{\sqrt{x^2+y^2+z^2}}$
$\hat{\boldsymbol{\varphi}}$	$-\dfrac{y}{\sqrt{x^2+y^2}}$	$\dfrac{x}{\sqrt{x^2+y^2}}$	0

Rectangular-spherical product in rectangular coordinates

Example: $\hat{\mathbf{x}}\cdot\hat{\mathbf{r}} = \sin\theta\cos\phi = \dfrac{x}{\sqrt{x^2+y^2+z^2}}$

Here are the transformations of vector components between coordinate systems:

Rectangular to cylindrical

$$A_r = A_x \frac{x}{\sqrt{x^2+y^2}} + A_y \frac{y}{\sqrt{x^2+y^2}}$$

$$A_\phi = -A_x \frac{y}{\sqrt{x^2+y^2}} + A_y \frac{x}{\sqrt{x^2+y^2}}$$

$$A_z = A_z$$

Cylindrical to rectangular

$$A_x = A_r \cos\varphi - A_\varphi \sin\varphi$$

$$A_y = A_r \sin\varphi + A_\varphi \cos\varphi$$

$$A_z = A_z$$

Rectangular to spherical

$$A_r = A_x \frac{x}{\sqrt{x^2+y^2+z^2}} + A_y \frac{y}{\sqrt{x^2+y^2+z^2}} + A_z \frac{z}{\sqrt{x^2+y^2+z^2}}$$

$$A_\theta = A_x \frac{xz}{\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}} + A_y \frac{yz}{\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}} - A_z \frac{\sqrt{x^2+y^2}}{\sqrt{x^2+y^2+z^2}}$$

$$A_\phi = -A_x \frac{y}{\sqrt{x^2+y^2}} + A_y \frac{x}{\sqrt{x^2+y^2}}$$

Spherical to rectangular

$$A_x = A_r \sin\theta\cos\phi + A_\theta \cos\theta\cos\phi - A_\phi \sin\phi$$

$$A_y = A_r \sin\theta\sin\phi + A_\theta \cos\theta\sin\phi + A_\phi \cos\phi$$

$$A_z = A_r \cos\theta - A_\theta \sin\theta$$

And here are expressions for the gradient, divergence, and curl in all three coordinate systems:

Rectangular coordinates

$$\nabla f = \hat{\mathbf{x}}\frac{\partial f}{\partial x} + \hat{\mathbf{y}}\frac{\partial f}{\partial y} + \hat{\mathbf{z}}\frac{\partial f}{\partial z}$$

$$\nabla \bullet \mathbf{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$$

$$\nabla \times \mathbf{A} = \hat{\mathbf{x}}\left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right) + \hat{\mathbf{y}}\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right) + \hat{\mathbf{z}}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix}$$

Cylindrical coordinates

$$\nabla f = \hat{\mathbf{r}}\frac{\partial f}{\partial r} + \hat{\boldsymbol{\varphi}}\frac{1}{r}\frac{\partial f}{\partial \phi} + \hat{\mathbf{z}}\frac{\partial f}{\partial z}$$

$$\nabla \bullet \mathbf{A} = \frac{1}{r}\frac{\partial}{\partial r}rA_r + \frac{1}{r}\frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z}$$

$$\nabla \times \mathbf{A} = \hat{\mathbf{r}}\left(\frac{1}{r}\frac{\partial A_z}{\partial \phi} - \frac{\partial A_\phi}{\partial z}\right) + \hat{\boldsymbol{\varphi}}\left(\frac{\partial A_r}{\partial z} - \frac{\partial A_z}{\partial r}\right) + \hat{\mathbf{z}}\frac{1}{r}\left(\frac{\partial}{\partial r}rA_\phi - \frac{\partial A_r}{\partial \phi}\right) = \begin{vmatrix} \hat{\mathbf{r}}\frac{1}{r} & \hat{\boldsymbol{\varphi}} & \hat{\mathbf{z}}\frac{1}{r} \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \phi} & \frac{\partial}{\partial z} \\ A_r & rA_\phi & A_z \end{vmatrix}$$

Spherical coordinates

$$\nabla f = \hat{\mathbf{r}}\frac{\partial f}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial f}{\partial \theta} + \hat{\boldsymbol{\varphi}}\frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}$$

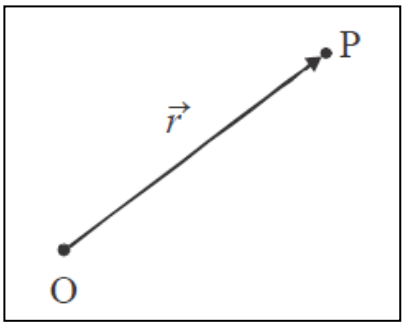
$$\nabla \bullet \mathbf{A} = \frac{1}{r^2}\frac{\partial}{\partial r}r^2A_r + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}(A_\theta \sin\theta) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial \phi}$$

$$\nabla \times \mathbf{A} = \hat{\mathbf{r}}\frac{1}{r\sin\theta}\left(\frac{\partial}{\partial \theta}(A_\phi \sin\theta) - \frac{\partial A_\theta}{\partial \phi}\right) + \hat{\boldsymbol{\theta}}\frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial A_r}{\partial \phi} - \frac{\partial}{\partial r}rA_\phi\right) + \hat{\boldsymbol{\varphi}}\frac{1}{r}\left(\frac{\partial}{\partial r}rA_\theta - \frac{\partial A_r}{\partial \theta}\right)$$

Velocity and acceleration in a different cooredinates systems{

First : Position vector:

It is a vector directed from some point to location of particle. In the figure shown r is position vector of particle 'P' with respect to point 'O'. If we specify the coordinate of particle then position vector can be expressed in terms of coordinates and unit vectors used in that coordinate system.



In cartesian coordinate system:

Coordinates of particle are written as (x, y, z) and unit vectors along x, y, z axes are $\hat{x}$, $\hat{y}$, and $\hat{z}$ respectively.

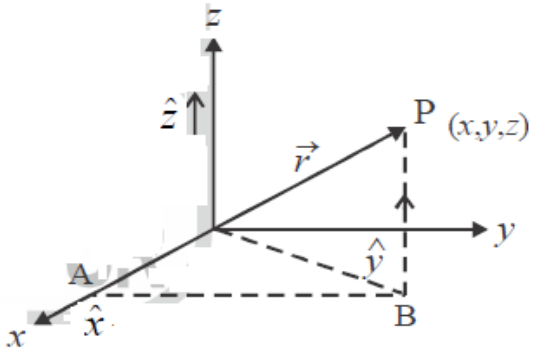
Therefoer, from figure,

$$OA = x,\ AB = y,\ BP = z$$

and $$\vec{OP} = \vec{OB} + \vec{BP}$$

$$\vec{r} = \vec{OA} + \vec{AB} + \vec{BP} = x\hat{x} + y\hat{y} + z\hat{z}$$

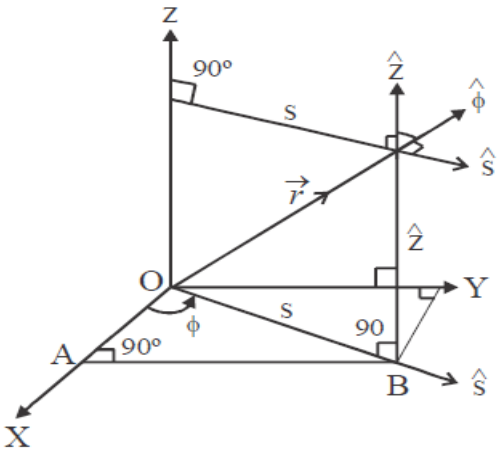
$$\therefore \quad \boxed{\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}}$$



Unit vectors are taken in the directions in which coordinates increase.

In cylindrical system

coordinates of particle are written as (s, φ, z) and unit vectors along the increasing direction of coordinates are ($\hat{s}$, $\hat{\varphi}$, $\hat{z}$). s is perpendicular distance of particle from z-axis, φ is its angular position with respect to x-axis and z is its distance above x-y plane.



Therefore, from figure $OB = s$, $\angle AOB =$, $BP = z$ and $\vec{OP} = \vec{OB} + \vec{BP}$

$$\boxed{\vec{r} = s\hat{s} + z\hat{z}}$$

relation with cartesian coordinates

$$\boxed{x = s\cos\phi,\ y = s\sin\phi,\ z = z} \quad \text{and} \quad \boxed{\hat{s} = \cos\phi\hat{x} + \sin\phi\hat{y},\ \hat{\phi} = -\sin\phi\hat{x} + \cos\phi\hat{y},\ z = \hat{z}}$$

In spherical polar coordinates system,

coordinates of particle are written as (r, ϑ, φ) and unit vector in increasing direction of coordinates are ($\hat{r}$, $\hat{\vartheta}$ and $\hat{\varphi}$), r is the distance of particle from origin, ϑ and φ are angular position with respect to z and x axes respectively.

From figure $OP = r$, $\angle COP = \theta$, $\angle AOB = \phi$ and $\vec{OP} = r\hat{r}$

$\therefore$ $\boxed{\vec{r} = r\hat{r}}$

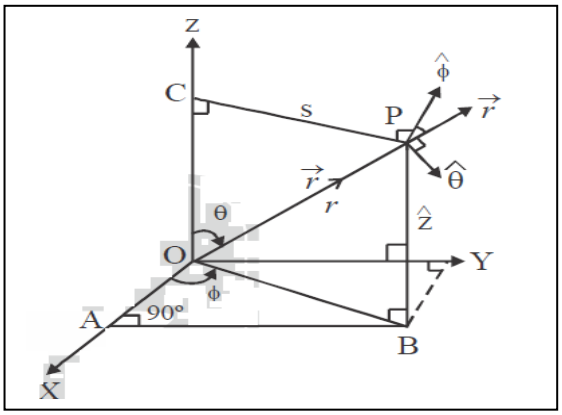
$OB = CP = r\sin\theta$, $BP = r\cos\theta$

$\therefore$ $AB = OB\sin\phi = r\sin\theta.\sin\phi$ and

$OA = OB\cos\phi = r\sin\theta\cos\phi$

Relation with cartesian coordinate,

$$\boxed{\mathbf{Z} = \cos\theta \quad \mathbf{y} = r\sin\theta\ \sin\phi \quad \mathbf{X} = r\sin\theta\cos\phi}$$



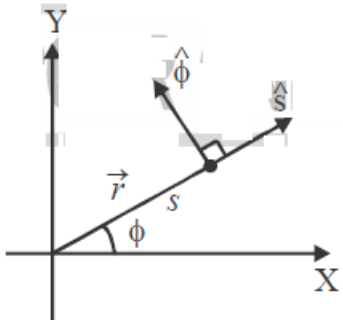
And $\hat{r} = \sin\theta\left(\cos\phi\hat{x} + \sin\phi\hat{y}\right) + \cos\theta\hat{z}$

$\hat{\theta} = \cos\theta\left(\cos\phi\hat{x} + \sin\phi\hat{y}\right) - \sin\theta\,\hat{z}$

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

If motion of a particle is confined in one plane then only two coordinates are required to describe its position.

We can either use cartesian coordinates (x, y) or plane polar coordinates (s, φ). Thus if a particle is moving on a plane then its position vector can be written as :



$$\vec{r} = x\hat{x} + y\hat{y}$$

Or, $$\vec{r} = s\hat{s} \text{ in (plane polar coordinate)}$$

Plane polar coordinates (s , ϕ) are the same coordinates which are used in cylindrical coordinates system.

Notice that, $\hat{x}$, $\hat{y}$ and $\hat{z}$ have a fixed direction as they are along the *x*, *y* and *z* axes, **whereas** $\hat{r}$, $\hat{s}$, $\hat{\vartheta}$, $\hat{\varphi}$ etc do not have fixed directions. **Therefore**, $\hat{x}$, $\hat{y}$, $\hat{z}$ are constant unit vectors **but** $\hat{r}, \hat{s}, \hat{\vartheta}, \hat{\varphi}$ **are not constant unit vectors.**

$$\text{Thus, } \frac{d\hat{x}}{dt} = 0, \frac{d\hat{y}}{dt} = 0, \frac{d\hat{z}}{dt} = 0 \text{ and } \frac{d\hat{r}}{dt} \neq 0, \frac{d\hat{s}}{dt} \neq 0, \frac{d\hat{\theta}}{dt} \neq 0, \frac{d\phi}{dt} \neq 0$$

Derivative of unit vectors $(\hat{r}, \hat{\vartheta}, \hat{s}, \hat{\varphi})$ can easily be found by using their relation with $(\hat{x}, \hat{y}, \hat{z})$.

For example: In plane polar or cylindrical coordinates,

$$\hat{s} = \cos\phi\hat{x} + \sin\phi\hat{y} \text{ and } \hat{\phi} = -\sin\phi\hat{x} + \cos\phi\hat{y}$$

Then:

$$\therefore \quad \frac{d\hat{s}}{dt} = -\sin\phi\frac{d\phi}{dt}\hat{x} + \cos\phi\frac{d\phi}{dt}\hat{y} = (-\sin\phi\hat{x} + \cos\phi\hat{y})\frac{d\phi}{dt} = \hat{\phi}\dot{\phi}$$

$$\text{and} \quad \frac{d\hat{\phi}}{dt} = -\cos\phi\frac{d\phi}{dt}\hat{x} - \sin\phi\frac{d\phi}{dt}\hat{y} = -(\cos\phi\hat{x} + \sin\phi\hat{y})\frac{d\phi}{dt} = -\hat{s}\dot{\phi}$$

$$\boxed{\frac{d\hat{s}}{dt} = \hat{\phi}\dot{\phi}, \qquad \frac{d\hat{\phi}}{dt} = -\hat{s}\dot{\phi}}$$

Second : Velocity (Average velocity is defined as) :

$$u_{av} = \frac{\text{total displacement}}{\text{total time taken}} = \frac{\text{change in position vector}}{\text{total time taken}} = \frac{r_2 - r_1}{t_2 - t_1}$$

Instantaneous velocity (velocity at any instant of time) is defined as time derivative of position vector.

Instantaneous velocity, $v = \frac{dr}{dt}$

By expersing (v) in different coordinate systems :

1- In Cartesian coordinate system :

$$r = x\hat{x} + y\hat{y} + z\hat{z}$$

Therefore, $$v = \frac{d}{dt}(x\hat{x} + y\hat{y} + z\hat{z}) = \frac{dx}{dt}\hat{x} + \frac{dy}{dt}\hat{y} + \frac{dz}{dt}\hat{z}$$

$$\boxed{\vec{v} = \dot{x}\hat{x} + \dot{y}\hat{y} + \dot{z}\hat{z}}$$

Or, $$v_x\hat{x} + v_y\hat{y} + v_z\hat{z}$$

$v_x = \dot{x} = \frac{dx}{dt}$ is component of velocity in x direction.

$v_y = \dot{y} = \frac{dy}{dt}$ is component of velocity in y direction

$v_z = \dot{z} = \frac{dz}{dt}$ is component of velocity in z direction

2- In plane coordinate system:

$$\vec{r} = s\hat{s}$$

Therefore, $\vec{v} = \frac{d}{dt}(s\hat{s}) = \frac{ds}{dt}\hat{s} + s\frac{d\hat{s}}{dt}$

$$\boxed{\vec{v} = \dot{s}\hat{s} + s\dot{\phi}\hat{\phi}} \qquad \left\{\because \frac{d\hat{s}}{dt} = \dot{\phi}\hat{\phi}\right\}$$

Or, $\vec{v} = v_s\hat{s} + v_\phi\hat{\theta}$

$v_s = \dot{s} = \frac{ds}{dt}$ is component velocity in $\hat{s}$ direction and it is called radial velocity

$v_\phi = s\dot{\phi} = s\frac{d\phi}{dt}$ is component velocity in $\hat{\phi}$ direction and it is called transverse velocity.

3- In cylindrical coordinate system:

$$\vec{r} = s\hat{s} + z\hat{z}$$

Therefore, $$\vec{v} = \frac{d\vec{r}}{dt} = \frac{d}{dt}(s\hat{s} + z\hat{z}) = \frac{ds}{dt}\hat{s} + s\frac{d\hat{s}}{dt} + \frac{dz}{dt}\hat{z}$$

$$\boxed{\vec{v} = \dot{s}\hat{s} + s\dot{\phi}\hat{\phi} + \dot{z}\hat{z}} \quad \textbf{where:} \quad \left\{\because \frac{d\hat{s}}{dt} = \dot{\phi}\hat{\phi}\right\}$$

Third : acceleration : Average acceleration is defined as

$$\vec{a}_{av} = \frac{\vec{v}_2 - \vec{v}_1}{t_2 - t_1}$$

Instantaneous acceleration is defined as time derivative of velocity vector.

$$\vec{a} = \frac{d\vec{v}}{dt}$$

By expressing v indifferent coordinatge system. We can writge acceleration of a particle in different coordi-nate system.

1- In cartesian coordinate:

$$\vec{v} = \dot{x}\hat{x} + \dot{y}\hat{y} + \dot{z}\hat{z}$$

Therefore, $$\vec{a} = \frac{d\vec{v}}{dt} = \frac{d}{dt}\left(\dot{x}\hat{x} + \dot{y}\hat{y} + \dot{z}\hat{z}\right)$$

$$\boxed{\vec{a} = \ddot{x}\hat{x} + \ddot{y}\hat{y} + \ddot{z}\hat{z}}$$

or, $$\vec{a} = \left(a_x\hat{x} + a_y\hat{y} + a_z\hat{z}\right)$$

$a_x = \ddot{x} = \frac{d}{dt}(\dot{x}) = \frac{dv_x}{dt}$ is component of acceleration along x-direction.

$a_y = \ddot{y} = \frac{d}{dt}(\dot{y}) = \frac{dv_y}{dt}$ is component of acceleration along y-direction.

$a_z = \ddot{z} = \frac{d}{dt}(\dot{z}) = \frac{dv_z}{dt}$ is component of acceleration along z-direction.

Since, $a_x = \frac{dv_x}{dt}$, therefore, if velocity along x-direction is constant then acceleration along x-direction must be zero.

2- In Plane polar coordinate :

$$\vec{v} = \dot{s}\hat{s} + s\dot{\phi}\hat{\phi}$$

Therefore, $$\vec{a} = \frac{d\vec{v}}{dt} = \frac{d}{dt}\left(\dot{s}\hat{s} + s\dot{\phi}\hat{\phi}\right)$$

$$= \ddot{s}\hat{s} + \dot{s}\frac{d\hat{s}}{dt} + \dot{s}\dot{\phi}\hat{\phi} + s\ddot{\phi}\hat{\phi} + s\dot{\phi}\frac{d\hat{\phi}}{dt}$$

$$= \ddot{s}\hat{s} + \dot{s}\left(\dot{\phi}\hat{\phi}\right) + \dot{s}\dot{\phi}\hat{\phi} + s\ddot{\phi}\hat{\phi} + s\dot{\phi}\left(-\dot{\phi}\hat{s}\right)$$

$$\boxed{\vec{a} = \left(\ddot{s} - s\dot{\phi}^2\right)\hat{s} + \left(2\dot{s}\dot{\phi} + s\ddot{\phi}\right)\hat{\phi}}$$

Or, $$\vec{a} = a_s\hat{s} + a_\phi\hat{\phi}$$

$a_s = \ddot{s} - s\dot{\phi}^2$ is component of acceleration along $\hat{s}$ and its called radial acceleration. Clearly, it is not equal to time derivative of radial component of velocity $(v_s = \dot{s})$.

Therefore, if v_S = constant , then a_S may not be zero.

$a_\phi = 2\dot{s}\dot{\phi} + s\ddot{\phi}$ is component of acceleration in $\hat{\phi}$ direction. It is called transverse acceleration. Clearly it is also not equal to time derivative of radial component of velocity $\left(v_\phi = s\dot{\phi}\right)$

i.e. $$a_\phi \neq \frac{d}{dt}\left(v_\phi\right)$$

Therefore, if v_φ= constant then a_φ may not be zero.

3-In cylindrical coordinate system:

$$\vec{v} = \dot{s}\hat{s} + s\dot{\phi}\hat{\phi} + \dot{z}\hat{z}$$

First two terms are same as in plane polar coordinate

Therefore, $$\vec{a} = \frac{d\vec{v}}{dt} = \left(\ddot{s} - s\dot{\phi}^2\right)\hat{s} + \left(2\dot{s}\dot{\phi} + s\ddot{\phi}\right)\hat{\phi} + \ddot{z}\hat{z}$$

****

Solved Problems

***Example* [1]:** A body moves in a spiral path in such a way that the radial distance decreases at a constant rate r = b – ct while the angular speed increases at a constant rate, , Find the speed as a function of time. By using equation of velocity

$$\mathbf{v} = \dot{r}\mathbf{e}_r + r\dot{\theta}\mathbf{e}_\theta$$

We have $\dot{r} = -c$ and $\ddot{r} = 0$.

$$\mathbf{v} = -c\mathbf{e}_r + (b - ct)kt\mathbf{e}_\theta$$

$$v = [c^2 + (b - ct)^2k^2t^2]^{1/2}$$

which is valid for $t \le b/c$. Note that $v = c$ both for $t = 0, r = b$ and for $t = b/c, r = 0$

***Example* [2]:** A particle is moving along a spiral path with its polar coordinate position r = bt2 and = ct where b and c is constant find the velocity and acceleration as a function of time. By using equation of velocity :

$$\mathbf{v} = \dot{r}\mathbf{e}_r + r\dot{\theta}\mathbf{e}_\theta$$

$$\begin{aligned} \mathbf{v} &= \mathbf{e}_r \frac{d}{dt}(bt^2) + \mathbf{e}_\theta (bt^2) \frac{d}{dt}(ct) \\ &= (2bt)\mathbf{e}_r + (bct^2)\mathbf{e}_\theta \end{aligned}$$

By using the equation of acceleration

$$\mathbf{a} = (\ddot{r} - r\dot{\theta}^2)\mathbf{e}_r + (r\ddot{\theta} + 2\dot{r}\dot{\theta})\mathbf{e}_\theta$$

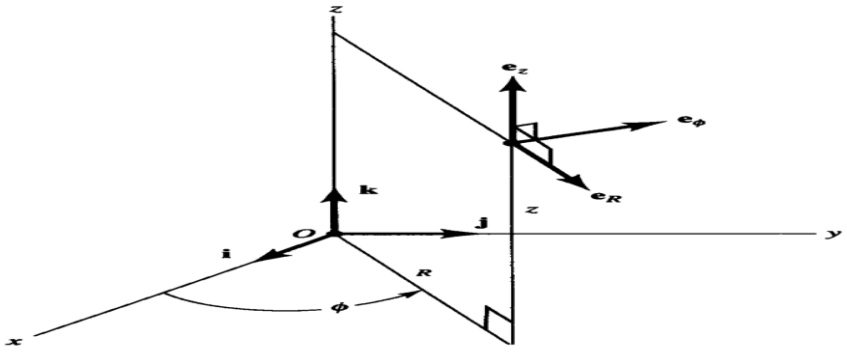
$$\begin{aligned} \mathbf{a} &= \mathbf{e}_r(2b - bt^2c^2) + \mathbf{e}_\theta[0 + 2(2bt)c] \\ &= b(2 - t^2c^2)\mathbf{e}_r + 4bct\mathbf{e}_\theta \end{aligned}$$

6. Velocity and Acceleration in Cylindrical Coordinates

In the case of three-dimensional motion, the position of a particle can be described in cylindrical coordinates R, , z. The position vector is then written as :

$$\mathbf{r} = R\mathbf{e}_R + z\mathbf{e}_z$$

Where e_R is a unit radial vector in the x-y plane and ez is the unit vector in the z direction. A third unit vector e_Φ is needed so that the three vectors e_R e_Φ ez constitute a right-handed triad,



The velocity and acceleration vectors are:

$$\mathbf{v} = \dot{R}\mathbf{e}_R + R\dot{\phi}\mathbf{e}_\phi + \dot{z}\mathbf{e}_z$$

$$\mathbf{a} = (\ddot{R} - R\dot{\phi}^2)\mathbf{e}_R + (2\dot{R}\dot{\phi} + R\ddot{\phi})\mathbf{e}_\phi + \ddot{z}\mathbf{e}_z$$

***Example* [3]:** A bead slides on a wire bent into the form of a helix, the motion of the bead being given in cylindrical coordinates by R = b, ⍰ = wt, z = ct. Find the velocity and acceleration vectors as functions of time.

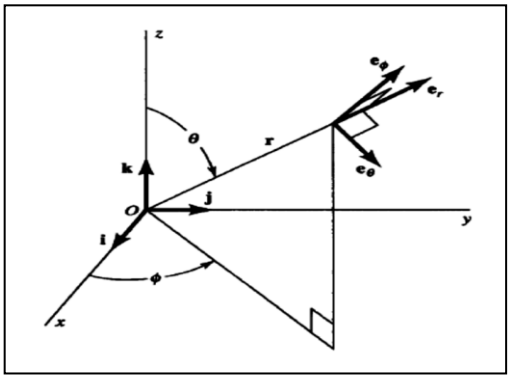
we find $\dot{R} = \ddot{R} = 0,\ \dot{\phi} = \omega,\ \ddot{\phi} = 0,\ \dot{z} = c,\ \ddot{z} = 0.$

$$\mathbf{v} = b\omega\mathbf{e}_\phi + c\mathbf{e}_z$$
$$\mathbf{a} = -b\omega^2\mathbf{e}_R$$

Fourth : Velocity and Acceleration in Spherical Coordinates

When spherical coordinates r,e, Φ are employed to describe the position of a particle, the position vector is written as the product of the radial distance r and the unit radial vector e_r, as with plane polar coordinates. Thus,

The velocity vector in terms of its components in the rotated triad.



$$\mathbf{v} = \mathbf{e}_r\dot{r} + \mathbf{e}_\phi r\dot{\phi}\sin\theta + \mathbf{e}_\theta r\dot{\theta}$$

The acceleration vector in terms of its components in the triad "

$$\mathbf{a} = (\ddot{r} - r\dot{\phi}^2\sin^2\theta - r\dot{\theta}^2)\mathbf{e}_r + (r\ddot{\theta} + 2\dot{r}\dot{\theta} - r\dot{\phi}^2\sin\theta\cos\theta)\mathbf{e}_\theta$$
$$+ (r\ddot{\phi}\sin\theta + 2\dot{r}\dot{\phi}\sin\theta + 2r\dot{\theta}\dot{\phi}\cos\theta)\mathbf{e}_\phi$$

Chapter (2)

Operators in Quantum Mechanics

Chapter (2)

Operators in Quantum Mechanics

1-POSTULATES OF QUANTUM MECHANICS

Postulate 1.

The state of a quantum mechanical system is completely specified by a function $\Psi(r, t)$ that depends on the coordinates of the particle(s) and on time. This function, called the wave function or state function, has the important property that $\Psi^*(r, t)\,\Psi(r, t)\,d\tau$ is the probability that the particle lies in $d\tau$ the volume element located at at **r** time **t** . The wavefunction must satisfy certain mathematical conditions because of this probabilistic interpretation. For the case of a single particle, the probability of finding it *3Tsomewhere3T* is 1, so that we have the normalization condition **:**

$$\int_{-\infty}^{\infty} \Psi^*(\mathbf{r}, t)\,\Psi(\mathbf{r}, t)\,d\tau = 1$$

It is customary to also normalize many-particle wavefunctions to 1.*0T*2*0T* The wavefunction must also be single-valued, continuous, and finite.

Postulate 2.

To every observable in classical mechanics there corresponds a linear, Hermitian operator in quantum mechanics.

This postulate comes about because of the considerations raised in section *0T*3.1.5*0T*: if we require that the expectation value of an operator is real, then must be a Hermitian operator. Some common operators occuring in quantum mechanics are collected in Table *0T*1*0T*.

*2T***Table 1:***2T* **Physical observables and their corresponding quantum operators (single particle)**

Table 1: Physical observables and their corresponding quantum operators (single particle)

Observation	Obs. Sympol	Operator Sympol	Operator
Position	$\underline{r}$	$\hat{\mathrm{r}}$	Multiply by $\underline{r}$
Momentum	p	$\hat{\mathrm{p}}$	$-i\hbar\left(\hat{i}\frac{\partial}{\partial x}+\hat{j}\frac{\partial}{\partial y}+\hat{k}\frac{\partial}{\partial z}\right)$
Kinetic energy	T	$\hat{T}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$
Hamiltonian	H	$\hat{H}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(\mathbf{r})$
Total energy	E	$\hat{E}$	$i\hbar\frac{\partial}{\partial t}$
Angular momentum	l_x	$\hat{l}_x$	$-i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)$
	l_y	$\hat{l}_y$	$-i\hbar\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)$
	l_z	$\hat{l}_z$	$-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)$

Postulate 3. In any measurement of the observable associated with operator $\hat{A}$, the only values that will ever be observed are the eigenvalues $\underline{a}$, which satisfy the eigenvalue equation

$$\hat{A}\Psi = a\Psi$$

This postulate captures the central point of quantum mechanics--the values of dynamical variables can be quantized (although it is still possible to have a continuum of eigenvalues in the case of unbound states). If the system is in an eigenstate of $\hat{A}$ with eigenvalue a, then any measurement of the quantity A will yield a.

Although measurements must always yield an eigenvalue, the state does not have to be an eigenstate of $\hat{A}$ *initially*. An arbitrary state can be expanded in the complete set of eigenvectors of $\hat{A}$ ($\hat{A}\Psi_i = a_i\Psi_i$) as

$$\Psi = \sum_i^n c_i \Psi_i$$

where n may go to infinity. In this case we only know that the measurement of A will yield *one* of the values a_i, but we don't know which one. However, we do know the *probability* that eigenvalue a_i will occur--it is the absolute value squared of the coefficient, $|c_i|^2$ (cf. section 3.1.4), leading to the fourth postulate below.

An important second half of the third postulate is that, after measurement of Ψ yields some eigenvalue a_i, the wavefunction immediately ``collapses" into the corresponding eigenstate Ψ_i (in the case that a_i is degenerate, then Ψ becomes the projection of Ψ onto the degenerate subspace). Thus, measurement affects the state of the system. This fact is used in many elaborate experimental tests of quantum mechanics.

Postulate 4. If a system is in a state described by a normalized wave function Ψ, then the average value of the observable corresponding to $\hat{A}$ is given by

$$< A >= \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi d\tau$$

Postulate 5. The wavefunction or state function of a system evolves in time according to the time-dependent Schrödinger equation

$$\hat{H}\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi}{\partial t}$$

The central equation of quantum mechanics must be accepted as a postulate, as discussed in section 2.2.

Postulate 6. The total wavefunction must be antisymmetric with respect to the interchange of all coordinates of one fermion with those of another. Electronic spin must be included in this set of coordinates.

The Pauli exclusion principle is a direct result of this *antisymmetry principle*. We will later see that Slater determinants provide a convenient means of enforcing this property on electronic wavefunctions.

Operators in Quantum Mechanics

Basic Concepts

• Operators are the principal components of quantum mechanics.

• Notationally, operators will be distinguished by **hats** on top of **symbols**.

• Every observable physical quantity, there exists a corresponding operator with real eigenvalues.

• In a finite number of dimensions, a matrix A can transform any arbitrary vector v into different vector $A\vec{v}$

$$\vec{v} \xrightarrow{Matrix\ A} \vec{\omega} = A\vec{v}$$

Similarly, an operator transforms a function into another function:

$$f(x) \xrightarrow{operator\ A} g(x) = Af(x)$$

Some simple examples of operators

$$f(x) \xrightarrow{\hat{x}} g(x) = xf(x)$$

$$f(x) \xrightarrow{\frac{d}{dx}} g(x) = xf(x)$$

- we say that the operator A is linear. If the action of an operator on a function $\Phi(x)$ is to multiply that function by some constant:

$$\hat{A}\Phi(x) = B\,\Phi(x)$$

we say that the constant B is an ***eigenvalue*** of the operator $\hat{A}$, and we call $\Phi(x)$ an **eigenfunction** of $\hat{A}$.

- In classical mechanics we work with the position X, the momentum P, the total energy E, etc. These quantities are called **dynamical variables**.
- In quantum mechanics the dynamical variables are no longer variables but **operators**.
- In physics or specially in quantum mechanics, to every observable quantity is associated a corresponding operator.
  - The position operator

$$\hat{x}f(x,y,z,t) = xf(x,y,z,t),$$
$$\hat{y}f(x,y,z,t) = yf(x,y,z,t),$$
$$\hat{z}f(x,,y,z,t) = zf(x,y,z,t)$$

  - The momentum operator

$$\hat{P} = -i\hbar\nabla.$$
$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x},\quad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}.\ \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$

  - The Hamiltonian operator $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

The Hamiltonian operator of a quantum mechanical system determines the evolutions of the system.

  - The energy operator $\hat{E} = i\hbar\frac{\partial}{\partial t}$
  - The kinetic energy operator $\hat{T} = -\frac{\hbar^2}{2m}\nabla$
  - The angular momentum operator

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right).\quad \hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right).\ \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

These operators are derived as the same, such as in the case of the classic mechanics for the particle and from the relation following

$$L = r \times p = \begin{vmatrix} i & j & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

An operator is a symbol which defines the mathematical operation to be carried out on a function

Examples of operators:

d/dx = first derivative with respect to x & $\sqrt{}$ = take the square root of & 3 = multiply by 3

Physical observables and their corresponding quantum operators (single particle)

كافة المشاهدات الفيزيائية (المقادير الفيزيائية،المتحولات الديناميكية)تمثل رياضيا بالمؤثرات، الجداول التالية يعطي أهم المتحولات الديناميكية في فضاء الموضع وكمية التحرك

Table 1 : First, Operators in space of position

Observation	Sympol of Obs.	operator Sympol	Operator in Quantum Mechanics
Position	$\underline{\mathbf{r}}$	$\hat{\mathbf{r}}$	Multiply by $\underline{\mathbf{r}}$
Momentum	p	$\hat{\mathrm{p}}$	$-i\hbar\left(\hat{i}\frac{\partial}{\partial x}+\hat{j}\frac{\partial}{\partial y}+\hat{k}\frac{\partial}{\partial z}\right)$
Kinetic energy	T	$\hat{T}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$
Potential energy	$V(\mathbf{r})$	$\hat{V}(\mathbf{r})$	Multiply by $V(\mathbf{r})$
Hamiltonian	H	$\hat{H}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(\mathbf{r})$
Total energy	E	$\hat{E}$	$i\hbar\frac{\partial}{\partial t}$
X^2	X^2	$\hat{x}^2$	$-\hbar^2\frac{\partial^2}{\partial p_x^2}$

Table 2: Second In Space Of Momentum

Observation	Sympol of Obs.	operator Sympol	Operator in Quantum Mechanics
Position	$\underline{r}$	$\hat{\mathbf{r}}$	$i\hbar\left(\hat{i}\frac{\partial}{\partial p_x}+\hat{j}\frac{\partial}{\partial p_y}+\hat{k}\frac{\partial}{\partial p_z}\right)$
Momentum	$\mathbf{p}$	$\hat{\mathbf{p}}$	$\hat{\mathbf{p}}$
Total energy	E	$\hat{E}$	$i\hbar\frac{\partial}{\partial t}$
X^2	X^2	$\hat{x}^2$	$-\hbar^2\frac{\partial^2}{\partial p_x^2}$

2- Basic Properties of Operators

- **Sum and subtract of two operators** :

$$(\hat{A}+\hat{B})f = \hat{A}f+\hat{B}f$$

$$(\hat{A}-\hat{B})f = \hat{A}f-\hat{B}f \qquad (2\text{-}1)$$

- **Multiple of two operators** :

$$\hat{A}\hat{B}f \equiv \hat{A}[\hat{B}f] \qquad (2\text{-}2)$$

- **For two equal operators** :

$$\hat{A}f = \hat{B}f \qquad (2\text{-}3)$$

- **Multiple of unit operator equal unity**:

$$\hat{1}f = f \qquad (2\text{-}4)$$

- **Mix law of operators** :

$$\hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C} \qquad (2\text{-}5)$$

- **Distribution law of operators** :

$$\hat{A}(\hat{B}+\hat{C}) = \hat{A}\hat{B} + \hat{A}\hat{C} \qquad (2\text{-}6)$$

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}$$

3- Linear Operators

The linear operators only are studied in quantum mechanicsand have the following properties :

$$\hat{A}(f+g) = \hat{A}f + \hat{A}g$$

$$\hat{A}(cf) = c\hat{A}f \qquad (3\text{-}1)$$

Where c is a constant value and both f & g are functions .

We apply the previous operators as : d/dxv, $()^2$, $\sqrt{}$ we find :

$$(d/dx)[cf(x)] = c\,(d/dx)f(x) \qquad (3\text{-}2)$$

linear operator

$$(f(x)+g(x))^2 \neq (f(x))^2 + (g(x))^2$$

$$\sqrt{\psi_1 + \psi_2} \neq \sqrt{\psi_1} + \sqrt{\psi_2} \qquad (3\text{-}3)$$

Two perators non linear

4- Eigenfunction /Eigenvalue Relationship :

When an operator operating on a function results in a constant times the function, the function is called an eigenfunction of the operator & the constant is called the eigenvalue

$$A\ f(x) = k\ f(x)$$

f(x) is the eigenfunction & k is the eigenvalue

Examples:-

Problem -1 : Prove that the following is eigenfunction,

$$\psi = A e^{-\alpha x}$$ for the following operator

$$\hat{F} = \frac{d^2}{dx^2} + \frac{2}{x}\frac{d}{dx} + \frac{2\alpha}{x}$$

Solusion

where A , α are constant

$$\hat{F}\psi = \frac{d^2}{dx^2}(Ae^{-\alpha x}) + \frac{2}{x}\frac{d}{dx}(Ae^{-\alpha x}) + \frac{2\alpha}{x}(Ae^{-\alpha x})$$

$$\hat{F}\psi = \alpha^2 Ae^{-\alpha x} + \frac{2}{x}(-\alpha Ae^{-\alpha x}) + \frac{2\alpha}{x}(Ae^{-\alpha x})$$

$$\hat{F}\psi = \left(\alpha^2 - \frac{2\alpha}{x} + \frac{2\alpha}{x}\right)Ae^{-\alpha x}$$

$$\hat{F}\psi = \alpha^2 Ae^{-\alpha x}$$

$$\hat{F}\psi = \alpha^2\psi$$

Then ψ is an eigenfunction and α^2 is an eigenvalue

Problem-2 **Find the eigenfunction for the following operator**

$$\hat{G} = -ih\frac{\partial}{\partial x} + bx$$

Problem (3) : Did the following function is an eigenfunction for the hamltonian operator

$$\psi = A\cos(kx - \omega t)$$

Solution

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U(x)\psi = i\hbar\frac{\partial}{\partial t}\psi$$

$$\nabla^2\psi = \frac{\partial^2}{\partial x^2}\psi(x,t) = -K^2\psi(x,t)$$

$$\frac{\partial}{\partial t}\psi(x,t) = -\omega A\sin(kx - \omega t) - \frac{\hbar^2}{2m}.-K^2\psi(x,t) + U(x)\psi(x,t)$$

$$= -i\hbar\omega A\sin(kx - \omega t)\ \frac{\hbar^2K^2}{2m}\psi(x,t) + U(x)\psi(x,t) = -i\hbar\omega A\sin(kx - \omega t)$$

$$\left(\frac{\hbar^2K^2}{2m} + U(x)\right)\psi(x,t) = -EiA\sin(kx - \omega t)$$

$$E\psi(x,t) = -EiA\sin(kx - \omega t) \Rightarrow \quad \psi(x,t) = -iA\sin(kx - \omega t) \neq A\cos(ks - \omega t)$$

الدالة لا تحقق الشرط

Problem (4) : $\frac{d2}{dx2}(sinax) =$, $\frac{d}{dx}(\frac{d}{dx}sinax) = (\frac{d}{dx}acosax)$

$= -a2sinax$ therefore

$sinax$ is Eigen function and $-a^2$ is Eigen value

Problem (5) : $\frac{d2}{dx2}(cosax) =$, $\frac{d}{dx}(\frac{d}{dx}cosax) = (\frac{d}{dx}asinax)$

$= -a2sinax$ therefore

$sinax$ is Eigen function and $-a^2$ is Eigen value

Problem (6) : explain if that's function $sin2x$ is Eigen function for the following mathematical operator $(cosx\frac{d3}{dx3})$,and $(tanx\frac{d3}{dx3})$,what is eigen values

if it's found.

Solution

$$cosx\frac{d3}{dx3}(sin2x) = cosx\frac{d2}{dx2}(\frac{d}{dx}sin2x) = 2cosx\frac{d}{dx}(\frac{d}{dx}sinxcosx)$$

$$= 2cosx\frac{d}{dx}(-sinx.sinx + cosx.cosx) = 2cosx\frac{d}{dx}(cos2x - sin2x)$$

$$= 2cosx(-2cosxsinx - 2cosx(2sinxcosx)$$

$$= -4cos2xsinx - 4cos2xsinx = -8cos2x.sinx$$

the function $sin2x$ is not eigen function for this mathematical operator.

Problem (7) :

$$tanx\frac{d3}{dx3}(sin2x) = tanx\frac{d2}{dx2}(\frac{d}{dx}sin2x)$$

$$= 2tanx\frac{d}{dx}(\frac{d}{dx}sinxcosx)$$

$$= 2tanx\frac{d}{dx}(-sinx.sinx + cosx.cosx)$$

$$= 2tanx\frac{d}{dx}(cos2x - sin2x)$$

$$= 2tanx(-2cosxsinx - 2tanx(2sinxcosx)$$

$$= -4\left(\frac{sinx}{cosx}\right).cosx.sinx - 4\left(\frac{sinx}{cosx}\right).cosx.sinx$$

$= -8sin2x$ the function $sin2x$ is eigen function for this mathematical operator and the eigen value is -8.

Home work:-

1- $\frac{d2}{dx2}$ for e^{-ax}

2- $cosx.\frac{d3}{dx3}$ for $cosx$

3- ∇^2 for cosax . cosby .coscz

4- $-h2/4\pi2(\frac{d2}{dx2}+cotx\frac{d}{dx})\,for\;\;3cos2x-1.$

5-أقواس التبادل والمبادلات Commutators in Quantum Mechanics :

If we have two operators $\hat{A}$, $\hat{B}$ have the same eigenfuction, then in this case we will have two eigenvalues a and b according to the two following equations :

بفرض لدينا مؤثرين $\hat{A}$, $\hat{B}$ لهما نفس الدالة المميزة(الخاصة) ،فحسب قواعد الدالة المميزة

والقيمة المميزة للمؤثر سيكون لدينا قيمتين مميزتين b,a وذلك وفق العلاقتين التاليتين:

$$\hat{A}\psi = a\psi$$
$$\hat{B}\psi = b\psi \qquad \textbf{(5-1)}$$

If we multply the first equation by $\hat{B}$ and the second equation by $\hat{A}$, we find :

$$\hat{B}\hat{A}\psi = a\hat{B}\psi$$
$$\hat{A}\hat{B}\psi = b\hat{A}\psi \qquad (5\text{-}2)$$

Because ψ is an eigenfunction for the two operators $\hat{A}$, $\hat{B}$, then we find

$$\hat{B}\hat{A}\psi = \hat{B}a\psi = ab\psi$$
$$\hat{A}\hat{B}\psi = \hat{A}b\psi = ba\psi \qquad (5\text{-}3)$$

By Substracting Equation two from equation one , we find :

$$\hat{B}\hat{A}\psi = ab\psi$$
$$\hat{A}\hat{B}\psi = ba\psi$$
$$\hat{A}\hat{B}\psi - \hat{B}\hat{A}\psi = b\ \psi - ab\psi$$
$$\left[\hat{A}\hat{B} - \hat{B}\hat{A}\right]\psi = [ba - ab]\psi$$
$$\left[\hat{A}\hat{B} - \hat{B}\hat{A}\right]\psi = [0]\psi \qquad (5\text{-}4)$$
$$\left[\hat{A}\hat{B} - \hat{B}\hat{A}\right]\psi = 0$$

Because the wave function ψ not equals zero, then the bracket equals zero, then:

$$\left[\hat{A}\hat{B} - \hat{B}\hat{A}\right] = 0 \qquad (5\text{-}5)$$ **then the two operators are comutators**

and the bracket is called the comutator bracket, ant it is one of the important relation in quantum mechanics. To measure or observe any two physical quantities at same time, its enough to brove the bracket of the two operators equals zero, or to prove the two operators are comutator , and if the comutator bracket ont equals zero , it means we can not able to measure the two physical quantities at the same time (uncertainty principale). Generally, the comutator bracket can be write as follow :

$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \qquad (5\text{-}6)$$

The following relations are important for comutations :

$$[\hat{A},\hat{B}] + [\hat{B},\hat{A}] = 0 \ \ \& \ \ [\hat{A},\hat{A}] = 0 \ \ \& \ \ [\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]$$
$$[\hat{A}+\hat{B},\hat{C}] = [\hat{A},\hat{C}] + [\hat{B},\hat{C}] \ \ \& \ \ [\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$$
$$[\hat{A}\hat{B},\hat{C}] = [\hat{A},\hat{C}]\hat{B} + \hat{A}[\hat{B},\hat{C}] \ \ \& \ \ \left[A_1A_2,B_1B_2\right] = B_1\left[A_1A_2,B_2\right] + \left[A_1A_2,B_2\right]B_2 \qquad (5\text{-}7)$$
$$[\hat{A},[\hat{B},\hat{C}]] + [\hat{C},[\hat{A},\hat{B}]] + [\hat{B},[\hat{C},\hat{A}]] = 0 \ \ \& \ \ [\hat{A},\hat{B}^n] = n\hat{B}^{n-1}[\hat{A},\hat{B}]$$
$$[\hat{A}^n,\hat{B}] = n\hat{A}^{n-1}[\hat{A},\hat{B}]$$

Exampls

$$[x,p^2] = [x,p]p + p[x,p] = i\hbar p + i\hbar p = 2i\hbar p$$

If you prefer to do it the long way around, you'll get the same answer:

$$[x,p^2]f(x) = -\hbar^2 x\frac{d^2f}{dx^2} + \hbar^2\frac{d^2}{dx^2}(xf) = -\hbar^2 x\frac{d^2f}{dx^2} + \hbar^2\frac{d}{dx}\left(x\frac{df}{dx} + f\right)$$

$$= -\hbar^2 x\frac{d^2f}{dx^2} + \hbar^2 x\frac{d^2f}{dx^2} + \hbar^2\frac{df}{dx} + \hbar^2\frac{df}{dx} = 2\hbar^2\frac{df}{dx} = 2i\hbar\left(-i\hbar\frac{df}{dx}\right) = 2i\hbar p f(x)$$

and therefore

$$[x,p^2] = 2i\hbar p$$

$$[2x^3,p] = 2[x^3,p]$$

(If you don't believe me you can leave it in, but you'll get the same answer.) If we let this commutator act on a test function $f(x)$, we get

$$[2x^3,p]f(x) = 2\left(-i\hbar x^3\frac{df}{dx} + i\hbar\frac{d}{dx}(x^3 f)\right)$$

$$= 2\left(-i\hbar x^3\frac{df}{dx} + i\hbar x^3\frac{df}{dx} + 3i\hbar x^2 f\right)$$

$$= 6i\hbar x^2 f(x)$$

and so, if we lose the test function, we find

$$[2x^3,p] = 6i\hbar x^2$$

$$\left[p_x, x^n\right]f(x) = p_x x^n f(x) - x^n p_x f(x)$$

$$\left[p_x, x^n\right]f(x) = -i\hbar\frac{d}{dx}x^n f(x) + i\hbar x^n\frac{df(x)}{dx}$$

$$\left[p_x, x^n\right]f(x) = -i\hbar n\,x^{n-1}f(x) - i\hbar x^n\frac{df(x)}{dx} + i\hbar x^n\frac{df(x)}{dx}$$

$$\left[p_x, x^n\right]f(x) = -i\hbar n\,x^{n-1}f(x)$$

we can solve the previous example by using the foolowing relations :

$$[\hat{A}^n, \hat{B}] = n\hat{A}^{n-1}[\hat{A}, \hat{B}]$$

$$[\hat{A}, \hat{B}^n] = n\hat{B}^{n-1}[\hat{A}, \hat{B}]$$

We find that :

$$\left[\hat{x}, \hat{p}^{n}\right] = np^{n-1}\left[\hat{x}, \hat{p}\right] = i\hbar n\hat{p}^{n-1}$$

$$\left[\hat{p}, \hat{x}^{n}\right] = nx^{n-1}\left[\hat{p}, \hat{x}\right] = -i\hbar n\hat{x}^{n-1}$$

$$\left[f(x), \hat{p}\right] = i\hbar\frac{\partial}{\partial x}f(x)$$

First , we must prove that :

$$\left[\hat{P}, \hat{H}\right] = 0$$

$$where \quad V(x) = 0$$

Second : we must prove that :

$$\hat{P}\psi = p\psi = \hbar k\psi$$

$$\hat{H}\psi = \frac{\hat{P}^2}{2m}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{dx^2}\psi = \frac{\hbar^2 k^2}{2m} = E\psi$$

Angular momentum Comutation operators

Comutation relations :

• Note : Angular momentum operators on different coordinates are not commutating :

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \quad \text{----------(1-1)}$$
$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

وبالمثل فإن :

$$\hat{L}^2 = \left|\hat{L}^2\right| = \hat{L}.\hat{L} = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \quad \text{----------(1-2)}$$

Or

$$\left|\vec{L}\right|^2 = \left|\vec{L}_x\right|^2 + \left|\vec{L}_y\right|^2 + \left|\vec{L}_z\right|^2$$
$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$
$$\hat{L}^2 = -\frac{h^2}{4\pi^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right],$$

$$\left[\hat{L}_x, \hat{L}_y\right] = \left[\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z\right]$$
$$\left[\hat{L}_x, \hat{L}_y\right] = \left[\hat{y}\hat{p}_z, \hat{z}\hat{p}_x\right] - \left[\hat{y}\hat{p}_z, \hat{x}\hat{p}_z\right] - \left[\hat{z}\hat{p}_y - \hat{z}\hat{p}_x\right] + \left[\hat{z}\hat{p}_y, \hat{x}\hat{p}_z\right]$$
$$\left[\hat{L}_x, \hat{L}_y\right] = \hat{y}\hat{p}_x\left[\hat{p}_z, \hat{z}\right] + \hat{x}\hat{p}_y\left[\hat{z}, p_z\right] = -i\hbar\hat{y}\hat{p}_x + i\hbar\hat{x}\hat{p}_y$$
$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\left[\hat{x}p_y - \hat{y}\hat{p}_x\right] \quad \text{----------(2)}$$
$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z \Rightarrow$$
$$\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x$$
$$\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$

While the total angular momentum operator commutating with all components of angular momentum on a coordinates, given the following relations :

$$\left[\hat{L}^2, \hat{L}_x\right] = 0$$
$$\left[\hat{L}^2, \hat{L}_y\right] = 0 \quad (3)$$
$$\left[\hat{L}^2, \hat{L}_z\right] = 0$$

Prove that:

$$\left[\hat{\phi}, \hat{L}_z\right] = i\hbar$$
$$\left[\sin\phi, \hat{L}_z\right] = i\hbar\cos\phi$$
$$\left[\nabla^2, \hat{L}_z\right] = 0$$

Simmalry;

وبالمثل فإن :

$$\hat{L}^2 = \left|\hat{L}^2\right| = \hat{L}.\hat{L} = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \text{ ----------(1-2)}$$

We begin to find commutating relations of angular momentum operators, and understand the role of commutation angular momentum operators in deriving these relations. .These operators gives the abslute values of these relations. Suppose a function f(x,y,z) and we need to prove that it is has a good behavioer (eigenfunction).

First : we need to determine the comutator $[\hat{L}_x, \hat{L}_y]$:

$$\hat{L}_y f = -i\hbar\left(z\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial z}\right) \text{ ----------(1-3)}$$

Multiply the last equationfrom lhe left side by the operator $\hat{L}_x$

نعامل المعادلة الأخيرة من اليسار بالمؤثر $\hat{L}_x$

$$\hat{L}_x\hat{L}_y f = -\hbar^2\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial z}\right)$$
$$= -\hbar^2\left[y\frac{\partial f}{\partial x} + yz\frac{\partial^2 f}{\partial z\partial x} - yx\frac{\partial^2 f}{\partial z^2} - z^2\frac{\partial^2 f}{\partial y\partial x} + zx\frac{\partial^2 f}{\partial y\partial z}\right] \quad (1-4)$$

Simelary, if we start by the operator $\hat{L}_x$

وبالمثل إذا ابتدأنا بالمؤثر $\hat{L}_x$ فإن :

$$\hat{L}_x f = -i\hbar\left(y\frac{\partial f}{\partial z} - z\frac{\partial f}{\partial v}\right) \quad (1-5)$$

$$\hat{L}_y\hat{L}_x f = -\hbar^2\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial f}{\partial z} - z\frac{\partial f}{\partial y}\right)$$
$$= -\hbar^2\left[zy\frac{\partial^2 f}{\partial x\partial z} - z^2\frac{\partial^2 f}{\partial x\partial y} - xy\frac{\partial^2 f}{\partial z^2} + x\frac{\partial f}{\partial y} + xz\frac{\partial^2 f}{\partial z\partial y}\right] \quad (1-6)$$

Using Eqs (1-5) & (1-6) , we get the comutation barcket $[\hat{L}_x, \hat{L}_y]$

$$\hat{L}_x\hat{L}_y f-\hat{L}_y\hat{L}_x f=-\hbar^2\left(y\frac{\partial f}{\partial x}-x\frac{\partial f}{\partial y}\right)$$

$$\left[\hat{L}_x,\hat{L}_y\right]=i\hbar\hat{L}_z \qquad (1-7)$$

We follow the same method to determine the comutators $\left[\hat{L}_y,\hat{L}_z\right]$, $\left[\hat{L}_z,\hat{L}_x\right]$

Eqs (1-1), show the periodic comutators operation. This means that replace y instead of x, and z instead by y, and z instead by x. This means that, if we carried out the periodic commutator on $\hat{L}_x$ we get $\hat{L}_y$ and simmlary the periodic commutator on $\hat{L}_y$ to get $\hat{L}_z$ and from $\hat{L}_z$ we can get $\hat{L}_x$ using the periodic commutating of cartezien coordinates , If we carried out the circular comutation on equation (1-7) .

Now we will find the commutation relations between $\hat{L}^2$ **and the three components** $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$

$$\left[\hat{L}^2,\hat{L}_x\right]=\left[\hat{L}_x^2+\hat{L}_y^2+\hat{L}_z^2,\hat{L}_x\right]=\left[\hat{L}_x^2,\hat{L}_x\right]+\left[\hat{L}_y^2,\hat{L}_x\right]+\left[\hat{L}_z^2,\hat{L}_x\right]$$
$$=\left[\hat{L}_y^2,\hat{L}_x\right]+\left[\hat{L}_z^2,\hat{L}_x\right]$$

حيث استخدمنا العلاقة (٣ - ١) . والآن وبتطبيق العلاقة (٨ - ١) فإن :

$$\left[\hat{L}^2,\hat{L}_x\right]=\left[\hat{L}_y,\hat{L}_x\right]\hat{L}_y+\hat{L}_y\left[\hat{L}_y,\hat{L}_x\right]+\left[\hat{L}_z,\hat{L}_x\right]\hat{L}_z+\hat{L}_z\left[\hat{L}_z,\hat{L}_x\right]$$
$$=-i\hbar\hat{L}_z\hat{L}_y-i\hbar\hat{L}_y\hat{L}_z+i\hbar\hat{L}_y\hat{L}_z+i\hbar\hat{L}_z\hat{L}_y=0$$

$$\left[\hat{L}^2,\hat{L}_x\right]=0 \qquad (1\text{-}10)$$

وبالمثل :

$$\left[\hat{L}^2,\hat{L}_y\right]=0 \quad ; \quad \left[\hat{L}^2,\hat{L}_z\right]=0 \qquad (1\text{-}11)$$

Exampe : Prove that $\left(\hat{L}_x\right)^\dagger=\hat{L}_x$

Solution

بأخذ المرافق للمؤثر $\hat{L}_x$ نجد أن:

$$\left(\hat{L}_x\right)^\dagger=\left(\hat{y}\hat{p}_z-\hat{z}\hat{p}_y\right)^\dagger$$
$$=\left(\hat{y}\hat{p}_z\right)^\dagger-\left(\hat{z}\hat{p}_y\right)=\hat{p}_z^\dagger\hat{y}^\dagger-\hat{p}_y^\dagger\hat{z}^\dagger=\hat{p}_z\hat{y}-\hat{p}_y\hat{z}$$
$$=\hat{y}\hat{p}_z-\hat{z}\hat{p}_y=\hat{L}_x$$

We have use the relations :

$$\left(\hat{A}+\hat{B}\right)^\dagger=\hat{A}^\dagger+\hat{B}^\dagger,\left(\hat{A}\hat{B}\right)^\dagger=\hat{B}^\dagger\hat{A}^\dagger$$

Example: Prove That :

$$\left[\hat{L}_x,\hat{L}_y\right]=\hat{L}_x\hat{L}_y-\hat{L}_y\hat{L}_x=i\hbar\hat{L}_z$$

Solution الحل: باستخدام تعريفات المؤثرات المعطاة، نجد أن:

By using the defintion of the operators , we get :

$$\left[\hat{L}_x,\hat{L}_y\right]=\left[\hat{y}\hat{p}_z-\hat{z}\hat{p}_y,\hat{z}\hat{p}_x-\hat{x}\hat{p}_z\right]$$

$$\left[\hat{L}_x,\hat{L}_y\right]=\left(\hat{y}\hat{p}_z-\hat{z}\hat{p}_y\right)\left(\hat{z}\hat{p}_x-\hat{x}\hat{p}_z\right)-\left(\hat{z}\hat{p}_x-\hat{x}\hat{p}_z\right)\left(\hat{y}\hat{p}_z-\hat{z}\hat{p}_y\right)$$

$$=\hat{y}\hat{p}_z\hat{z}\hat{p}_x-\cancel{\hat{y}\hat{p}_z\hat{x}\hat{p}_z}-\cancel{\hat{z}\hat{p}_y\hat{z}\hat{p}_x}+\hat{z}\hat{p}_y\hat{x}\hat{p}_z$$

$$-\hat{z}\hat{p}_x\hat{y}\hat{p}_z+\cancel{\hat{z}\hat{p}_x\hat{z}\hat{p}_y}+\cancel{\hat{x}\hat{p}_z\hat{y}\hat{p}_z}-\hat{x}\hat{p}_z\hat{z}\hat{p}_y$$

$$=\hat{y}\hat{p}_z\hat{z}\hat{p}_x+\hat{z}\hat{p}_y\hat{x}\hat{p}_z-\hat{z}\hat{p}_x\hat{y}\hat{p}_z-\hat{x}\hat{p}_z\hat{z}\hat{p}_y$$

$$=\hat{y}\hat{p}_x\left(\hat{p}_z\hat{z}-\hat{z}\hat{p}_z\right)+\hat{p}_y\hat{x}\left(\hat{z}\hat{p}_z-\hat{p}_z\hat{z}\right)$$

$$=i\hbar\left(-\hat{y}\hat{p}_x+\hat{p}_y\hat{x}\right)$$

$$=i\hbar\hat{L}_z \qquad \text{(هـ . ط . ث)}$$

Another method using comutation laws, we get :

$$\left[\hat{L}_x,\hat{L}_y\right]=\left[\hat{y}\hat{p}_z-\hat{z}\hat{p}_y,\hat{L}_y\right]$$

$$=\hat{y}\underbrace{\left[\hat{p}_z,\hat{L}_y\right]}_{I}+\underbrace{\left[\hat{y},\hat{L}_y\right]}_{=0}\hat{p}_z-\hat{z}\underbrace{\left[\hat{p}_y,\hat{L}_y\right]}_{=0}+\underbrace{\left[\hat{z},\hat{L}_y\right]}_{II}\hat{p}_y$$

Where;

$$=\left[\hat{p}_z,\hat{L}_y\right]=\left[\hat{p}_z,\left(\hat{z}\hat{p}_x-\hat{x}\hat{p}_z\right)\right]$$

$$=\left[\hat{p}_z,\hat{z}\hat{p}_x\right]-\left[\hat{p}_z,\hat{x}\hat{p}_z\right]$$

$$=\hat{z}\underbrace{\left[\hat{p}_z,\hat{p}_x\right]}_{=0}+\underbrace{\left[\hat{p}_z,\hat{z}\right]}_{=-i\hbar}\hat{p}_x-\hat{x}\underbrace{\left[\hat{p}_z,\hat{p}_z\right]}_{=0}+\underbrace{\left[\hat{p}_z,\hat{x}\right]}_{=0}\hat{p}_z=$$

$$=-i\hbar\hat{p}_x .$$

And ,

$$II = \left[\hat{z}\,,\hat{L}_y\right] = \left[\hat{z}\,,(\hat{z}\hat{p}_x - \hat{x}\hat{p}_z)\right]$$
$$= \left[\hat{z}\,,\hat{z}\hat{p}_x\right] - \left[\hat{z}\,,\hat{x}\hat{p}_z\right]$$
$$= \hat{z}\underbrace{\left[\hat{z}\,,\hat{p}_x\right]}_{=0} + \underbrace{\left[\hat{z}\,,\hat{z}\right]}_{=0}\hat{p}_x - \hat{x}\underbrace{\left[\hat{z}\,,\hat{p}_z\right]}_{=-i\hbar} + \underbrace{\left[\hat{z}\,,\hat{x}\right]}_{=0}\hat{p}_z$$
$$= -i\hbar\hat{x}$$

Finally, we find :

$$\left[\hat{L}_x\,,\hat{L}_y\right] = \hat{y}\,(-i\hbar\hat{p}_x) - (-i\hbar\hat{x})\,\hat{p}_y$$
$$= i\hbar\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right)$$
$$= i\hbar\hat{L}_z \qquad \text{(هـ . ط. ث)}$$

Orthogonality and Normalization conditions

6-Orthogonality and Normalization (Orthonormalization) condition شرط التنظيم(المعايرة) والتعامد

The probapility of finding a particle in any place in volume dv as a wave function , given by the following relation :

$$dp = |\psi(r,t)|^2 dv = \psi^*(r,t)\psi(r,t)dv \qquad (6\text{-}1)$$

حيث dp يعطي احتمال تواجد الإلكترون في الحجم dv ويأخذ دوما قيما حقيقية، هذا وان احتمال تواجد الجسيم فى كامل الفضاء المدروس يفرض تكامل العلاقة السابقة فنجد:

$$p = \int_{-\infty}^{+\infty} dp = \int_{-\infty}^{+\infty} |\psi(r,t)|^2 dv = 1 \qquad (6\text{-}2)$$

This relation gives the probapility of finding the particle in all space equals 100 % = 1 , and the relation which varifay this condition is called the normalization condition.

وفي حال كون الدالة منظمة(معايرة) فان شرطي التنظيم والتعامد يعطيا وفق العلاقة:

$$\int \psi_n \psi_m dv = \delta_{nm}$$

$$when \quad n = m \Rightarrow \int \psi_n \psi_m dv = \delta_{nm} = 1$$

$$when \quad n \neq m \Rightarrow \int \psi_n \psi_m dv = \delta_{nm} = 0 \qquad (6\text{-}3)$$

وفي حال عدم تحقق شرط المعايرة نضرب التكامل بثابت ما بحيث يتحقق شرط المعايرة أي:

$$A^2 \int \psi_n \psi_m dv = \delta_{nm}$$

$$when \quad n = m \Rightarrow A^2 \int \psi_n \psi_m dv = \delta_{nm} = 1$$

$$when \quad n \neq m \Rightarrow A^2 \int \psi_n \psi_m dv = \delta_{nm} = 0 \qquad (6\text{-}4)$$

$$\psi(r) = \sum_i b_i u_i(r)$$

where b_i is the distributer factor, and we can get it from multiblying **the above Eqs from both sides in the conjegate of the eigenfunction** u_p **and then by integration, we get**

حيث b_i معامل النشر ويمكن الحصول علية من ضرب العلاقة السابقة من الطرفين بمرافق الدالة المميزة u_n ثم المكاملة وفق العلاقة التالية:

$$\int u_n^*(r)\psi(r)dv = \sum_i b_i \int u_n^* u_i(r)dv = \sum_i b_i \delta_{ni} = b_n \qquad (6\text{-}7)$$

The probabiblity, to get the eigenvalues a_n **for the studied operator**

إن احتمال الحصول على القيم الخاصة a_n للمؤثر المدروس تعطى بالعلاقة:

$$\wp(a_n) = \left|\int u_n^*(r)\psi(r)dv\right|^2 = \left|\sum_i b_i \int u_n^* u_i(r)dv\right|^2 = \left|\sum_i b_i \delta_{ni}\right|^2 = b_n^2 \qquad (6\text{-}8)$$

أمثلة:جسيم داخل بئر جهد لانهائي عرضه a له الدالة التالية المستقلة عن الزمن والغير معايرة:

$$\psi(x) = A \sin\frac{\pi n}{a}x$$

Find the normalized constant A , where :

$$\sin^2\theta = \frac{1-\cos 2\theta}{2} \quad \text{and,} \quad \cos^2\theta = \frac{1+\cos 2\theta}{2}$$

Solution

Using the normalization condition, we find

باستخدام شرط التنظيم(المعايرة) تابع الحل

$$\int_0^a |\psi(x)|^2 dx = \int_0^a \left| A \sin\frac{\pi n}{a}x \right|^2 dx = 1 \Rightarrow$$

$$A^2 \int_0^a \sin^2\frac{\pi n}{a}x\, dx = A^2 \int_0^a \left(\frac{1-\cos\frac{2\pi n}{a}x}{2} \right) dx = 1$$

$$A^2 \left(\int_0^a \frac{1}{2} dx \right) - \int_0^a \frac{\cos\frac{2\pi n}{a}x}{2} dx = 1$$

$$A^2 . \frac{a}{2} - 0 = 1 \Rightarrow A^2 = \frac{2}{a} \Rightarrow A = \sqrt{\frac{2}{a}}$$

$$then \qquad \psi(x) = \sqrt{\frac{2}{a}} \sin\frac{\pi n}{a}x$$

وهذه الدالة الأخيرة معايرة جرب بنفسك بتطبيق علاقة المعايرة من جديد

Example-3 : A particle exisiting in space and it is limited by (oo x < -oo), and it is descriped by the wave function :

$$\psi(x,t) = A\, e^{-x^2}\, e^{i(kx-\omega t)}$$

1- Normalized constant (A)

2- Probapility of finding the particle in any position between (,), If we know that

$$\int_0^\infty e^{-\alpha x^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}$$

First, A is a normlized constant. and we can get the normlization condition by integrating the square function, and ثابت المعايرةA:شرط المعايرة تكامل مربع الدالة يساوي الواحد ومنه

$$\Psi(\mathbf{x},\mathbf{t}) = \mathbf{A}e^{-x^2}e^{i(kx-wt)}$$

$$\int_{-\infty}^{+\infty}\left|\mathbf{A}e^{-x^2}e^{i(kx-wt)}\right|^2 dx = 1$$

$$\mathbf{A}^2\int_{-\infty}^{+\infty}\left|\mathbf{e}^{-x^2}e^{i(kx-wt)}\right|^2 dx = 1$$

$$\mathbf{A}^2\int_{-\infty}^{+\infty}\left|\mathbf{e}^{-x^2}\left\{e^{i(kx-wt)}\right\}\right|^2 dx = 1$$

$$2\mathbf{A}^2\int_{0}^{+\infty}\mathbf{e}^{-2x^2}\left|\left\{e^{i(kx-wt)}\right\}\right|^2 dx = 1$$

$$2\mathbf{A}^2\int_{0}^{+\infty}\mathbf{e}^{-2x^2}\left|\left\{e^{-i(kx-wt)}e^{i(kx-wt)}\right\}\right|dx = 1$$

$$2\mathbf{A}^2\left(\frac{1}{2}\sqrt{\frac{\pi}{2}}\right) = 1 \Rightarrow A^2 = \sqrt{\frac{\pi}{2}}^{-1} \Rightarrow A = \sqrt{\sqrt{\frac{\pi}{2}}^{-1}}$$

Second, The probability of finding the particle in the separation (x, x+dx)

$$dp = |\psi(r,t)|^2 dv = \psi^*(r,t)\psi(r,t)dv$$

$$dp = \sqrt{\frac{\pi}{2}}^{-1}\left|\mathbf{e}^{-x^2}e^{i(kx-wt)}\right|^2 dx$$

$$dp = \sqrt{\frac{\pi}{2}}^{-1}e^{-2x^2}dx$$

Third : Total probability :

$$p = \int_{-\infty}^{+\infty}\left|\sqrt{\sqrt{\frac{\pi}{2}}^{-1}}\,\mathbf{e}^{-x^2}e^{i(kx-wt)}\right|^2 dx$$

$$p = \sqrt{\frac{\pi}{2}}^{-1}\int_{-\infty}^{+\infty}\left|\mathbf{e}^{-x^2}e^{i(kx-wt)}\right|^2 dx$$

$$p = \sqrt{\frac{\pi}{2}}^{-1}\int_{-\infty}^{+\infty}\mathbf{e}^{-2x^2}e^{\pm i(kx-wt)}dx$$

$$p = \sqrt{\frac{\pi}{2}}^{-1}\int_{-\infty}^{+\infty}\mathbf{e}^{-2x^2}dx$$

$$p = \sqrt{\frac{\pi}{2}}^{-1} 2\int_0^{+\infty} \mathbf{e}^{-2x^2} dx = \sqrt{\frac{\pi}{2}}^{-1} 2.\frac{1}{2}\sqrt{\frac{\pi}{2}} = 1$$

Example :

Particle move in a potential field $-a \le x \le a$ Find the normalized constant for the following its wave function : .

$$\psi(x) = A \cos\frac{\pi}{2a}x$$

In most cases, we go and useing which is called prpbability density , given by

$$\rho(r,t) = \frac{|\psi(r,t)|^2}{\int_{-\infty}^{+\infty} \psi^*(r,t)\psi(r,t)d\ v}$$

$$\int_{-\infty}^{+\infty} \rho(r,t)dv = 1$$

7- The expectation value القيمة المتوقعة

In quantum mechanics , all information about the studied particle are exists in its wavefuction , and from it we get the probability of finding the particle in any place through any time. The expectation values for the physical quantity is the title of this statment.

Classically, to calculate the expectation vale for any observation such as the position , we suppose that the studied case contains N number of particles . There are N_i particle exsist at X_i .

The mean value for the particle position given by :

كلاسيكيا لحساب القيمة المتوقعة لمشاهدة ما ولتكن الموضع ،يفترض أن الجملة المدروسة مؤلفة من N جسيم منها N_i جسيم موجود في الموقع X_i ،فالقيمة الوسطية لموقع الجسيم تعطى بالعلاقة التالية:

$$\bar{X} = \frac{N_1X_1 + N_2X_2 + \ldots\ldots + N_mX_m}{N_1 + N_2 + \ldots\ldots + N_m}$$

$$\bar{X} = \frac{\sum_i N_iX_i}{\sum N_i} \qquad (7\text{-}1)$$

In quantum mechanics , for one particle , then for finding a particle at X_i and probability P_i and the expectation for the particle position is :

وكميا من أجل جسيم واحد فان تواجد الجسيم في الموضع X_i سيكون باحتمال p_i والقيمة المتوقعة لموضع الجسيم هو:

$$\bar{X} = \frac{p_1 x_1 + p_2 x_2 + ... + p_m x_m}{p_1 + p_2 + ... + p_m} = \frac{\sum_i p_i x_i}{\sum_i p_i} \qquad (7\text{-}2)$$

The probability given by :

$$p_i = |\psi_i|^2 dx \qquad (7\text{-}3)$$

وفي حال كون الجملة مستمرة يحول المجموع السابق إلى تكامل:

$$\bar{x} = \frac{\int x |\psi|^2 dx}{\int |\psi|^2 dx} = \langle x \rangle \qquad (7\text{-}4)$$

When the wave function is normalized and eigenfunction for the operator $\hat{A}$, then expectation value equation for the physical quantity as before given by :

وعندما تكون الدالة الموجية معايرة ودالة خاصة للمؤثر $\hat{A}$ ،عندئذ تكون معادلة القيم الذاتية للمقدار الفيزيائي كما سبق وأعطيت كالتالي :

$$\hat{A}\psi(r) = a\psi(r) \qquad (7\text{-}5)$$

إن القيمة الخاصة a للمؤثر هي ما نقصد به القيمة المتوقعة لحالة نقية ويمكن استنتاجها بضرب العلاقة السابقة من الطرفين ومن اليسار بمرافق الدالة الموجية ثم المكاملة على كامل الفضاء فنجد:

$$\int \psi^*(r)\hat{A}\psi(r)dv = \int \psi^*(r)a\psi(r)dv = a$$

$$then \quad \langle A \rangle = \int \psi^*(r)\hat{A}\psi(r)dv = a \qquad (7\text{-}6)$$

وهي علاقة القيمة المتوقعة أو القيمة الوسطى للمقدار الفيزيائي المدروس وفي حال كون الدالة الموجية

It is like a linear strcture for many eigenfunction , so we write the general expression for the expectation value for physical quantity as follow : عبارة عن تركيب خطي لعدة دوال خاصة فإننا نكتب العبارة العامة للقيمة المتوقعة لأي مقدار فيزيائي بالشكل التالي:

$$\langle A \rangle = \frac{\int_{-\infty}^{+\infty} \psi^* \hat{A} \psi dv}{\int_{-\infty}^{+\infty} \psi^* \psi dv} \qquad (7\text{-}7)$$

If the wavefunction is normalized, then the integration in the the domeator of the relation equals unity

Expectation value and Eigenvalue of Operators

- The expectation value of a random variable is a concept from probability. In quantum mechanics, a measurable quantity or an observable in the real world is a random variable. For each observable in the real world, there is a corresponding operator in the quantum world.
- The relation between the classical value of an observable and its quantum mechanical counterpart, the operator, is via the expectation relation, viz.,

$$\langle \hat{A} \rangle = \int_{-\infty}^{+\infty} \psi^*(r) \hat{A} \psi(r)\, dr$$

The above reduces to a scalar number. It is also the bridge between classical quantities and quantum mechanical entities.

- This is expectation value or mean of an operator $\hat{A}$ with respect to the wave function $\psi(r)$.
- The mean value of an operator is not necessarily a value that can actually be measured. So it may not turn out to be equal to one of the eigenvalues of $\hat{A}$.
- The expectation value of an operator for a quantum system in state f is defined to be:

$$\langle \hat{A} \rangle = \langle f | \hat{A} | f \rangle$$

- This expectation value can be written in term of the eigenstate and eigenvalues of $\hat{A}$ as:

$$\langle \hat{A} \rangle = \sum_n \sum_m \langle \psi_n | \hat{A} | \psi_m \rangle \, f_n^* f_m$$

When ψ_m is the eigenstate of $\hat{A}$ with eigenvalue A_m, the above can be written as:

$$\langle \hat{A} \rangle = \sum_n \sum_m \langle \psi_n | \hat{A} | \psi_m \rangle \, f_n^* f_m = \sum_n A_n |f_n|^2$$

where $|f_n|^2$ is the probability of finding the state in eigenstate n. Hence, the above is the statistical average or the expectation value of the eigenvalue A_n . The eigenvalue A_n can be thought of as a random variable.

8 -combination of eigenstates مبدأ تراكب الحالات

If the wave function is a linear constrction of several eigenfunction for any operator, then the expectation mean value of the studied physical quantityis given by following wavefunction

نعود إلى مسألة كون الدالة الموجية كتركيب خطي لعدة دوال خاصة لمؤثر ما ولنحاول إيجاد القيمة المتوقعة للمقدار المدروس،تعطى الدالة الموجية في هذه الحالة بالعلاقة:

$$\psi = c_1\psi_1 + c_2\psi_2 + \ldots\ldots + c_i\psi_i = \sum_{i=1}^{N} c_i\psi_i \qquad (8\text{-}1)$$

for calculating the expectation value for physical quantity is given by the expectation values relation, then the wave function consider normalized :

ولنحسب القيمة المتوقعة لمتحول ديناميكي(مقدار فيزيائي) من علاقة القيم المتوقعة ونعتبر الدالة معايرة

$$\langle A \rangle = \int \psi^* \hat{A} \psi dv$$

$$\langle A \rangle = \int \left[\sum_{i=1}^{N} c_i \psi_i \right]^* \hat{A} \left[\sum_{j=1}^{N} c_j \psi_j \right] dv$$

$$\langle A \rangle = \sum_{i=1}^{N} c_i^* \sum_{j=1}^{N} c_j \int \psi_i^* \hat{A} \psi_j dv$$

$$c_i^* = c_i$$

$$\langle A \rangle = \sum_{i=1}^{N} c_i \sum_{j=1}^{N} c_j \int \psi_i^* a_j \psi_j dv$$

$$\langle A \rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} c_i c_j a_j \int \psi_i^* \psi_j dv$$

$$\langle A \rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} c_i c_j a_j \delta_{ij}$$

$$when \quad i = j$$

$$\langle A \rangle = \sum_{i=1}^{N} c_i^2 a_i \qquad (8\text{-}2)$$

Note : the expectation valuefor each staterelated by the probability as given by :

لاحظ أن القيمة المتوقعة لكل حالة ترتبط ألان بالاحتمال الذي درسناه سابقا في العلاقة:

$$p(a_n)=\left|\int u_n^*(r)\psi(r)dv\right|^2=\left|\sum_i b_i\int u_n^* u_i(r)dv\right|^2=\left|\sum_i b_i\delta_{ni}\right|^2=b_n^2 \qquad (8\text{-}3)$$

The propability for geting the absolute a must be the propability given by square C

أى أن احتمال الحصول على القيمة a_i يكون باحتمال مساوى إلى c_i^2 .

Example

If we have eigen function for any operator given by:

لديك دالة موجية خاصة لمؤثر ما تعطى بالعلاقة التالية:

$$\psi = c_1\psi_1 + c_3\psi_3$$

Example -1: Find the expectation value for the following :
Genarally, the expectation value given by the following relation:

$$\langle A\rangle=\frac{\sum_{i=1}^{N}c_i^2a_i}{\sum_{i=1}^{N}c_i^2}=\frac{c_1^2a_1+c_3^2a_3}{c_1^2+c_3^2}$$

$$\langle A\rangle=\frac{c_1^2a_1}{c_1^2+c_3^2}+\frac{c_3^2a_3}{c_1^2+c_3^2}$$

$$where \qquad p=\sum_i c_i^2=c_1^2+c_3^2=1$$

$$\langle A\rangle=c_1^2a_1+c_3^2a_3$$

فلو كان المقدار هو الطاقة سيكون لدينا مستويي طاقة أحدهما $a_1=E_1$ والأخر $a_3=E_3$

القيمة المتوقعة الأولى ستكون باحتمال c_1^2 والثانية باحتمال c_3^2 وبشكل عام يكون احتمال أي قياس مفرد معطى بالعلاقة:

$$p_i=\frac{|c_i|^2}{\sum_i c_i^2}$$

Example-2 :

Particle in a rigd wall box move in one dimension -x , and a is the width of the box . if the wavefunction of the moving particle at the time t = 0 is :

$$\psi(x,0) = \frac{3\phi_2 + 4\phi_9}{\sqrt{25}}$$

Find the following :

1- Did the wave function of the moving particle is normalized ?.

2-Find the gian energy values , and the probability of finding these energy values : أوجد قيم الطاقة التي يمكن الحصول عليها وبأي احتمال نجد كل من هذه القيم؟

Solusion

1- The first request :

$$\int \psi^* \psi dx = \int \left(\frac{3\phi_2 + 4\phi_9}{\sqrt{25}}\right)\left(\frac{3\phi_2 + 4\phi_9}{\sqrt{25}}\right) dx$$

$$\int \psi^* \psi dx = \int \frac{9\phi_2\phi_2}{25} dx + \int \frac{12\phi_2\phi_9}{25} dx + \int \frac{12\phi_9\phi_2}{25} + \int \frac{16\phi_9\phi_9}{25}$$

$$\int \psi^* \psi dx = \frac{9}{25} + \frac{16}{25} = \frac{25}{25} = 1$$

2- The second request :

$$c_i = 0 \quad except \quad i = 2,9 \neq 0 \Leftrightarrow c_2 = \frac{3}{\sqrt{25}}, c_9 = \frac{4}{\sqrt{25}}$$

$$p_i = \frac{|c_i|^2}{\sum_i c_i^2} \Rightarrow \sum_i c_i^2 = c_2^2 + c_9^2 = \frac{9}{25} + \frac{16}{25} = 1 \Rightarrow$$

$$p_i = |c_i|^2$$

$$p_2(E_2) = c_2^2 = \frac{9}{25}$$

$$p_9(E_9) = c_9^2 = \frac{16}{25}$$

$$p_{i\neq 2,9}(E_{i\neq 2,9}) = 0$$

Expectation values of energy :

$$\langle E \rangle = c_2^2 E_2 + c_9^2 E_9$$

$$\langle E \rangle = \frac{9}{25} E_2 + \frac{16}{25} E_9$$

إن هذا الجسيم لديه احتمالان للتواجد إما في المستوي الطاقي الثاني وباحتمال 9\25 = 36%أو في المستوي الطاقي التاسع وباحتمال 16\25=64%، وبمعنى آخر لو كان لدينا 25 صندوق كل منها يحوي جسيم في نفس الشروط السابقة تماما فان 9 جسيمات ستشغل المستوي الطاقي الثاني ،و 16 جسيم ستشغل المستوي التاسع.

Example-3 :

Find the expectation value of the moving particle momentum on x-axes.

$$\langle p_x \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{p}_x \psi dx = \int_{-\infty}^{+\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi dx$$

$$\langle p_x \rangle = -i\hbar \int_{-\infty}^{+\infty} \psi^* \frac{\partial}{\partial x} \psi dx$$

$$\langle p_x \rangle = -i\hbar \int_{-\infty}^{+\infty} \psi^* \frac{\partial}{\partial x} A e^{i(k_x x - \omega t)} dx$$

$$\langle p_x \rangle = -i\hbar . ik_x \int_{-\infty}^{+\infty} \psi^* \psi dx = \hbar k_x$$

Example-4 : Find the expectation values of the energy ?

$$\langle E \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{E} \psi dx = \int_{-\infty}^{+\infty} \psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \psi dx$$

$$\langle E \rangle = i\hbar \int_{-\infty}^{+\infty} \psi^* \frac{\partial}{\partial t} \psi dx$$

$$\langle E \rangle = i\hbar \int_{-\infty}^{+\infty} \psi^* \frac{\partial}{\partial t} A e^{i(k_x x - \omega t)} dx$$

$$\langle E \rangle = i\hbar . -i\omega \int_{-\infty}^{+\infty} \psi^* \psi dx = \hbar\omega$$

Example-5 : Find the expectation value for both $\hat{p}^2, \hat{H}$? .

The uncertenaty principal of the positon and momentum for particle are conected directily by the expectation values according to the absolute measuring error in experiments, the gian error in any measuring given by the foolowing relations

يرتبط عدم التعيين (اللاتحديد)في موقع الجسيم (Δx) وكمية حركته (Δp_x) بالقيم المتوقعة مباشرة فوفقا لقياسات الخطأ المطلق في التجارب فان الخطأ المرتكب في قياس ما يعطى وفقا للعلاقات التالية:

إن الشك في قياس A و B يحدد كما يلي:

$$\Delta A^2 = \langle A^2 \rangle - \langle A \rangle^2 \Rightarrow \Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$

$$\Delta B^2 = \langle B^2 \rangle - \langle B \rangle^2 \Rightarrow \Delta B = \sqrt{\langle B^2 \rangle - \langle B \rangle^2}$$

Then , the certanity in measuring two values given by :

$$(\Delta A)(\Delta B) \geq \frac{1}{2}| < C > |$$

وهذه هي علاقة مبدأ الشك الشهيرة لهايزنبرغ والتي يمكن اشتقاقها من أجل الموضع وكمية الحركة

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

xample-5: If the wave function of the particle :

$$\psi = A e^{i(\kappa_x x - \omega t)}$$

1- Prove that the uncertienty in particle posion equal infinity ∞ ?

$$\langle p_x \rangle = \hbar k_x \Rightarrow \langle p_x \rangle^2 = \hbar^2 k_x^2$$

we find,

The solution as we see in previous example

Also , we find :

$$\langle p_x^2 \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{p}_x \psi dx = \int_{-\infty}^{+\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right)^2 \psi dx$$

$$\langle p_x^2 \rangle = -\hbar^2 \int_{-\infty}^{+\infty} \psi^* \frac{\partial^2}{\partial x^2} \psi dx$$

$$\langle p_x^2 \rangle = -\hbar^2 \int_{-\infty}^{+\infty} \psi^* \frac{\partial^2}{\partial x^2} A e^{i(k_x x - \omega t)} dx$$

$$\langle p_x^2 \rangle = -\hbar^2 . - k_x^2 \int_{-\infty}^{+\infty} \psi^* \psi dx = \hbar^2 k_x^2$$

By applying the uncerteinty principal for measuring the momentum, we find :

$$\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = \sqrt{\hbar^2 k_x^2 - \hbar^2 k_x^2} = 0$$

$$\Delta p_x . \Delta x \geq \frac{\hbar}{2} \Rightarrow \Delta x \geq \frac{\hbar}{2\Delta p_x} = \frac{\hbar}{0} = \infty$$

9 Hermitian Operators المؤثرات الهرميتية

All physical observations are represented by the expectation values, and the value of physical observation must be real (Energy, Momentum, Density, ...) , this means the following relation must be varified :

$$\langle A \rangle = \langle A \rangle^*$$

$$\int \psi^* \hat{A} \psi dx = \int (\hat{A}\psi)^* \psi dx = \left[\int (\hat{A}\psi) \psi^* dx \right]^* \quad (9\text{-}1)$$

The operator which varify this condition is called hermitian operator, it must varify the following relation :

Example-5 :

If the wavefunction of the paricle given by :

$$\langle A\rangle = \int \psi^* \hat{A}\psi dv = \int \left(\hat{A}\psi\right)^* \psi dv = \langle A\rangle^*$$

$$\langle A\rangle = \int \psi^* a\psi dv = \int (a\psi)^* \psi dv = \int a^*\psi^*\psi dv = \langle A\rangle^*$$

$$\langle A\rangle = a\int \psi^*\psi dv = a^*\int \psi^*\psi dv = \langle A\rangle^* \qquad (9\text{-}2)$$

$$\langle A\rangle = a = a^* = \langle A\rangle^*$$

In Case of two wave functions have the same operator , then we have two cases varifying :

First : Orthegonal condition :

$$\int \psi_1^* \hat{A}\psi_2 dv = \int \left(\hat{A}\psi_1\right)^* \psi_2 dv$$

$$\int \psi_1^* a_2\psi_2 dv = \int (a_1\psi_1)^* \psi_2 dv$$

$$a_2\int \psi_1^*\psi_2 dv - a_1^*\int \psi_1^*\psi_2 dv = 0$$

$$(a_2 - a_1^*)\int \psi_1^*\psi_2 d \Rightarrow (a_2 - a_1^*)\delta_1 = 0$$

$$when \quad i \neq j \Rightarrow \delta_{12} = 0 \qquad (9\text{-}3)$$

$$then \quad (a_2 - a_1^*) = (a_2 - a_1) \neq 0$$

$$\Rightarrow \int \psi_1^*\psi_2 dv = \delta_{12} = 0$$ وهو شرط التعامد من شرط الهرميتية

Second : Normalization condition

$$\int \psi_1^* \hat{A}\psi_2 dv = \int \left(\hat{A}\psi_1\right)^* \psi_2 dv$$

$$\int \psi_1^* a_2\psi_2 dv = \int (a_1\psi_1)^* \psi_2 dv$$

$$a_2\int \psi_1^*\psi_2 dv - a_1^*\int \psi_1^*\psi_2 dv = 0$$

$$(a_2 - a_1^*)\int \psi_1^*\psi_2 d \Rightarrow (a_2 - a_1^*)\delta_1 = 0$$

$$when \quad i = j \Rightarrow \delta_{12} = 1$$

$$then \quad (a_2 - a_1^*) = (a_2 - a_1) = 0 \qquad (9\text{-}4)$$

$$\Rightarrow a_1 = a_2 = a$$

$$\Rightarrow \int \psi_1^*\psi_2 dv = \delta_{12} = \delta_{11} = 1$$ وهو شرط التنظيم من شرط الهرميتية

Chapter (3)

Shrodenger's Equations

3-1: Introduction to wavefunction

During 1925 three different but equivalent versions of quantum theory were proposed. Schrödinger-proposed wave mechanics; Heisenberg-developed matrix mechanics and Dirac introduced operator theory.

Considering the de Broglie's matter waves Erwin Schrödinger, an Austrian physicist, argued that if a particle like an electron behaves as a wave then the equation of wave motion could be successfully applied to it. He postulated a function varying in both space and time in a wavelike manner (hence called wave function and denoted it as ψ). This function is generally complex and assumed to contain information about a system.

Schrödinger set up a linear and time-dependent wave-like equation, called Schrödinger wave equation, to describe the wave aspect of a particle taking account of de Broglie's relation for wavelength. Physically, $|\psi(X,\ t)|^2$, where $\psi(X,\ t)$ is the solution of the Schrödinger equation, is interpreted as position probability density. That is, $|\psi(X,\ t)|^2$ is the probability density of observing a particle at position X at time t. ψ does not give exact outcomes of observations but helps us to know all possible events and their probabilities. Further, the probability interpretation allows us to find the average or expected result of a set of measurements on a quantum system.

3-2: The wavefunction

In classical mechanics : Determination of the position for any microscopic particle at any time (i.e. $x(t)$) leads to find any other interested dynamical variables velocity ($v = dx\ /\ dt$), the momentum ($p = mv$),the kinetic energy [$KE = (1/2)\ mv^2$], etc.

In Quantum Mechanics : The information about the state of a particle is described by a ***wavefunction,*** which is usually denoted by $\psi(r,t)$ and can be used to describe all dynamical variables (i.e. velocity (v), the momentum (p),the kinetic energy (KE).

This wavefunction can take various formula, the sinusoidal wave is the simplest example of a periodic continuous wave and can be used to build more complex waves.

$$\vec{\psi}(\vec{r}.t) = \vec{\psi}_o sin(\vec{k}\cdot\vec{r} - \omega t + \phi)$$

This sinusoidal wave can be written with exponential form as:

$$\vec{\psi}(\vec{r}.t) = \psi_o \cdot e^{-i(\vec{k}\cdot\vec{r}-\omega t+\phi)}$$

Exponential form ⇔ sin/cos form

$$\vec{\psi}_o sin(\vec{k}\cdot\vec{r}\mp\omega t) = \vec{\psi}_o \frac{1}{2j}\left[e^{j(\vec{k}\cdot\vec{r}\mp\omega t)} - e^{-j(\vec{k}\cdot\vec{r}\mp\omega t)}\right]$$

$$\vec{\psi}_o cos(\vec{k}\cdot\vec{r}\mp\omega t) = \vec{\psi}_o \frac{1}{2j}\left[e^{j(\vec{k}\cdot\vec{r}\mp\omega t)} + e^{-j(\vec{k}\cdot\vec{r}\mp\omega t)}\right]$$

Wave Travelling (1D)

$$\frac{\partial^2}{\partial x^2}\vec{\psi} = \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\vec{\psi},\ v = \frac{1}{\sqrt{\mu\varepsilon}}$$

There are several interesting features of the wave function ψ.

• The **probability** interpretation of $|\psi|2$ imposes certain conditions on meaningful ψ. Further, the $|\psi|^2$ satisfies a conservation law, an equation analogous to the continuity equation of flow in hydrodynamics.

• To set the total probability unity the ψ must satisfy the **normalization** condition

Knowing ψ we can compute **expectation values** of variables such as position, momentum, etc.

• In quantum mechanics the experimentally measurable variables are no longer dynamical variables but they become **operators**. The outcomes of experiments are the eigenvalues of the operators of the observables.

• A valid wavefunction must be "well behaved," with specific properties

➢ Single valued of the parameters of the system.

➢ Continuous and finite.

➢ Differentiable.

➢ Square integrable.

➢ Space coordinate and time.

Q1:-Wave Function

If $\psi(x) = \frac{N}{x^2+a^2}$, calculate the normalization constant N.

Solution:-

Normalization condition is

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1$$

$$N^2 \int_{-\infty}^{+\infty} (x^2 + a^2)^{-2} dx = 1$$

Put $x = a\tan\theta; dx = sec2\theta\, d\theta$

$$\left(\frac{2N^2}{a^3}\right)\int_0^{\pi/2} cos^2\theta d\theta = N^2\pi/2a^3 = 1$$

Therefore,

$$N = \left(\frac{2a^3}{\pi}\right)^{1/2}$$

Q2.Wave Function

Let $\psi(x) = Ae^{-|x|/2a}e^{i(x-x_o)}$. Find the constant A by normalizing the wavefunction.

Solution:-

$$\psi^*(x) = Ae^{-|x|/2a}e^{-i(x-x_o)}$$

$$\psi^*(x)\,\psi(x) = |A|^2 e^{-|x|/2a}e^{-i(x-x_o)}e^{-|x|/2a}e^{i(x-x_o)}$$

$$= |A|^2 e^{-|x|/a}e^{-i(x-x_o)}e^{i(x-x_o)}$$

$$= |A|^2 e^{-|x|/a}$$

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2\, dx = |A|^2 \int_{-\infty}^{0} e^{x/a} + |A|^2 \int_0^{\infty} e^{-x/a}$$

Let $u = x/a$, then $du = dx/a$.

$$\int_{-\infty}^{0} e^{x/a}\, dx = a\int_{-\infty}^{0} e^u du = ae^{x/a}|_{-\infty}^{0} = a[e^0 - e^{-\infty}] = a[1-0] = a$$

Application of the same technique to the second term also gives a.

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2\, dx = |A|^2 \int_{-\infty}^{0} e^{x/a} + |A|^2 \int_0^{\infty} e^{-x/a} = A^2a + A^2a = 2A^2a$$

Using the normalization condition:

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

We obtain

$$A = \frac{1}{\sqrt{2a}}$$

The normalized wavefunction is then:

$$\psi(x) = \frac{1}{\sqrt{2a}} e^{-|x|/2a} e^{i(x-x_o)}$$

Q3:-Wave Function

Find the flux of particles represented by the wave function

$$\psi(x) = A\, e^{ikx} + Be^{-ikx}$$

Solution:-

The flux is

$$J_x = \left(\frac{\hbar}{2im}\right)\left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right]$$

$$J_x = \left(\frac{\hbar}{2im}\right)\left[(A\, e^{-ikx} + Be^{ikx})ik(A\, e^{ikx} - Be^{-ikx}) + (A\, e^{ikx} + Be^{-ikx})ik(A\, e^{-ikx} + Be^{ikx})\right]$$

$$J_x = \left(\frac{\hbar k}{2m}\right)\left[A^2 - B^2 - ABe^{-2ikx} + \mathrm{ABe^{2ikx}} + \mathrm{A^2} - \mathrm{B^2} + \mathrm{ABe^{-2ikx}} - \mathrm{ABe^{2ikx}}\right] = \left(\frac{\hbar \mathrm{k}}{\mathrm{m}}\right)[\mathrm{A^2} - \mathrm{B^2}]$$

• The Probability Interpretation and Normalization :

The Born's statistical interpretation of the wave function has been used to describe the state of particle, which says that $|\Psi(x.\ t)|^2$ gives the probability of finding the particle at point x, at time t - or more precisely;

$$|\Psi(x.t)|^2 dx = \begin{pmatrix}\text{probability of finding the particle}\\ \text{between } x \text{ and } (x+dx). \text{at time } t\end{pmatrix}$$

The statistical interpretation introduces a kind of indeterminacy into QM and because of the statistical interpretation, probability plays a control role in QM. For example, when an electron manifests as a wave, it is described by :

$$\psi(z) \propto exp(ikz) \qquad \text{and} \qquad \frac{\partial^2}{\partial z^2}\psi(z) = -k^2\psi(z)$$

And a generalization of this wave into three dimensions' yields :

$$\nabla^2\psi(r) = -k^2\psi(r)$$

The statistical interpretation of the wave function $|\Psi(x.\ t)|^2$ is the probability density for finding the particle at point x at time t.The value of the integral of the probability density must be equal 1, so that the particle's go to be somewhere :

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

This mathematical relation represents the normalization of the probability density for finding the particle over all region.

III. The Schrödinger's wave Equation

Schrödinger in 1924 provided a formulation called wave mechanics which incorporated

- The principle of quanta (Planck).
- Wave -particle duality (de Broglie).

Based on the wave-particle duality principle, we will describe the motion of electron in a crystal by wavefunction $\Psi(r.t)$.

Classical physics

$$\frac{p^2}{2m} + V(x) = E$$

Wave mechanics

$$p \longrightarrow -i\hbar\frac{\partial}{\partial x} \qquad E \rightarrow i\hbar\frac{\partial}{\partial t}$$

The behavior of a particle of mass m subject to a potential $V\ (x,t)$ is described by the following partial differential equation that named as "**Schrödinger's wave Equation**" المعادلة العامة لشرودينجر

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x.t)}{\partial x^2} + V(x)\Psi(r.t) = i\hbar\frac{\partial\Psi(r.t)}{\partial t}$$

I- The Time-dependent Schrodinger equation derivative :

The wave function $\Psi(x.t)$ of a particle moving in x-direction in terms of p_x and E can be expressed as:

$$\Psi(r.t) = A\exp\left[-i\left(\frac{Et}{\hbar} - \frac{p_x x}{\hbar}\right)\right] \qquad (1)$$

From this equation

$$\frac{\partial\Psi}{\partial t} = -\frac{iE}{\hbar}\Psi \qquad (2)$$

$$i\hbar\frac{\partial\Psi}{\partial t} = E\Psi \qquad (3)$$

$$\frac{\partial\Psi}{\partial x} = \frac{ip_x}{\hbar}\Psi \qquad (4)$$

$$-i\hbar\frac{\partial\Psi}{\partial x} = p_x\Psi \qquad (5)$$

Differentiating Eq. 1, again with respect to x, we have

$$-i\hbar\frac{\partial^2\Psi}{\partial x^2} = p_x\frac{\partial\Psi}{\partial x} = i\frac{{p_x}^2}{\hbar}\Psi \qquad (6)$$

$$-\hbar^2\frac{\partial^2\Psi}{\partial x^2} = {p_x}^2\Psi \qquad (7)$$

For a non-relativistic free particle, the total energy E of the particle moving in x -direction is equal to its kinetic energy T.

$$E = T = \frac{{p_x}^2}{2m}$$

Multiplying both sides of above equation by Ψ, we have

$$E\Psi = \frac{{p_x}^2}{2m}\Psi \qquad (8)$$

Making use of Eqs. (2) and (7) we can write Eq. (8) as:

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} \qquad (9)$$

This equation is known as time-dependent Schrödinger for a free particle. If the particle is moving in a force field described by potential energy function **V**, its total energy is

$$E = \frac{{p_x}^2}{2m} + V$$

and the Schrödinger equation, it will be now in the form of

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \qquad (10)$$

in three dimensions, it is represented by:

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2\Psi + V\Psi \qquad (11)$$

is known as the time-dependent Schrödinger equation of a particle in three dimensions.

The Schrödinger equation is motivated by further energy balance that total energy is equal to the sum of potential energy and kinetic energy. Defining the potential energy to be V (r), the energy balance equation becomes

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\Psi(r.t) = E\Psi(r.t)$$

However, it predicts many experimental outcomes, as well as predicting the existence of *electron orbitals inside an atom*, and *how electron would interact with other particles*.

II- Stasionary State (Time-independent Schrodinger Equation)

When the potential energy V is independent of time, the wave function may be written as product of two wave functions, of which one is function of x and the other is function of t only Assume the position and time parameters in wavefunction is separable.

$$\Psi(r.t) = \psi(r)\phi(t) \qquad in\ 3D$$

or

$$\Psi(x.t) = \psi(x)\phi(t) \qquad in\ 1D$$

The Schrödinger equation Eq. (10) can be written with this new form of the wavefunction as

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

Divided the equation above be $\psi(x)\phi(t)$ we get

$$\frac{-\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}$$

The left side of equation is a function of position x only and the right side is a function of time t only, which implies each side of this equation must be equal to same constant.

$$\frac{-\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = \eta\ (constant)$$

iii. Physical meaning of η

$$i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = \eta\ (constant)$$

$\Rightarrow\ \phi(t) = e^{-i(\eta/\hbar)t} = e^{-i\omega t}$ The position-independent wavefunction is always in a form of exponential term $e^{-i\omega t}$.

Where $\frac{\eta}{\hbar} = \omega$

$\because E = \hbar\omega \ \Rightarrow \eta = E$ The separation constant is the total energy E of the particle.

Whereas, the wave equation can be written as $\Psi(x.t) = \psi(x)\phi(t) = \psi(x)\,e^{-i\omega t}$

Then we can find two solutions to the time-independent Schrödinger equation:

$$\frac{-\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = E$$

Or

$$\frac{-\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) - E = 0$$

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0$$

Case 1: $k = \frac{2m[E-V(x)]}{\hbar^2} > 0$ if $E > V(x) \Rightarrow \psi(x) = A\exp(\pm ikx)$

Case 2: $\gamma = \frac{2m[V(x)-E]}{\hbar^2} > 0$ if $V(x) > E \Rightarrow \psi(x) = A\exp(\pm i\gamma x)$

iv. Physical meaning of the wave equation

- $\Psi(x.t)$ cannot be a physical wave like an oscillating string, or EM wave of Maxwell theory.
- TDSE is complex equation, solutions are inherently complex (real and imaginary parts of Ψ do not separately solve equation)
- Something that is complex cannot be directly measured.
- Max Born postulated in 1926 that the wavefunction $|\Psi(x.t)|^2dx$ is the probability of finding the particle between x and dx at a given

$$\begin{aligned}|\Psi(x.t)|^2 &= \Psi(x.t)\cdot\Psi(x.t)^*\\ &= \psi(x)e^{-i(E/\hbar)t}\cdot\psi(x)^*e^{+i(E/\hbar)t}\\ &= \psi(x)\cdot\psi(x)^*\end{aligned}$$

Probability $|\Psi(x.t)|^2 = \psi(x) \cdot \psi(x)^*$

- The probability density function is independent of time.
- Fortunately, the Schrödinger equation has the property that it automatically preserves the normalization of the wave function.

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x.t)|^2dx = \int_{-\infty}^{+\infty}\frac{\partial}{\partial t}|\Psi(x.t)|^2dx$$

[Note that the integral is a function only of x, so we use a total derivative ($\frac{d}{dt}$) in the first term, but the integrand is a function of x as well as t, so it's partial derivative ($\frac{\partial}{\partial t}$) in the second one].

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi$$

Now the Schrödinger equation says that

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi$$

And hence (taking the complex conjugate of equation above)

$$\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*$$

So

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right) = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right]$$

The integral of equation above can be now evaluated explicitly by the equation:

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x.t)|^2dx = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)\Big|_{-\infty}^{+\infty}$$

But $\Psi(x.t)$ must go to zero as x goes to ($\mp$) infinity – otherwise the wave function would not be normalizable. It follows that

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x.t)|^2dx = 0$$

And hence that the integral on the left is constant (independent of time); if Ψ is normalize at $t = 0$, it stays normalize for all future time.

- The state of a particle has to be more richly endowed and described by a wave function or state function $\Psi(x, t)$. The state function (also known as a state vector) is a vector in the infinite dimensional space.
- The state of a particle in quantum mechanics is described by a state function, which has infinitely many degrees of freedom.

- In the Schrödinger equation, the wave function $\Psi(x, t)$ is a continuous function of the position variable x at any time instant t; hence, it is described by infinitely many numbers, and has infinite degrees of freedom.

v. Boundary condition for wavefunction

- The probability of finding the particle over the entire space must be equal to 1

$$\int_{-\infty}^{+\infty} |\Psi(x.t)|^2 dx = \int_{-\infty}^{+\infty} \psi(x) \cdot \psi(x)^* dx = 1$$

- $\psi(x)$ must be finite, single-valued and continuous.
- $\partial\psi(x)/\partial x$ must be finite, single-valued and continuous.
- If the probability were to become infinite at some point in space, then the probability of finding the particle at the position would be certain, that violate the uncertainty principle.
- The second derivative must finite which implies that the first derivative must be continuous.
- The first derivative is related to the particle momentum, which must be finite and single-valued.
- The finite first derivative implies that the function itself must be continuous.

vi. Probabilistic Interpretation of the wave function

The final, most accepted interpretation of this wave function (one that also agrees with experiments) is that its magnitude squared corresponds to the probabilistic density function. In other words, the probability of finding an electron in an interval $[x;\ x + \Delta x]$ is equal to

$$|\Psi(x.t)|^2\ \Delta x$$

For the 3D case, the probability of finding an electron in a small volume ΔV in the vicinity of the point r is given by

$$|\Psi(x.t)|^2\ \Delta V$$

Since the magnitude squared of the wavefunction represents a probability density function, it must satisfy the normalization condition of a probability density function, viz.,

$$\int |\Psi(x.t)|^2\ \mathrm{d}V = 1$$

The magnitude squared of this wave function is like some kind of "energy" that cannot be destroyed. Electrons cannot be destroyed and hence, charge conservation is upheld by the Schrödinger equation.

Motivated by the conservation of the "energy" of the wave function, we shall consider an "energy" conserving system where the classical Hamiltonian will be a constant of motion. In this case, there is no "energy" loss from the system. Therefore, the Schrödinger equation that governs the time evolution of the wave function is:

$$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \qquad (1)$$

where $\hat{H}$ is the Hamiltonian operator, one can solve (1) formally to obtained:

$$\Psi(t) = e^{-i\frac{\hat{H}}{\hbar}t}\Psi(t=0) \qquad (2)$$

Since the above is a function of an operator, it has meaning only if this function acts on the eigenvectors of the operator $\hat{H}$. It can be shown easily that if $\bar{A} \cdot V_i = \lambda_i V_i$,

$$exp(\bar{A}) \cdot V_i = exp(\lambda_i)\ V_i \qquad (3)$$

If $\hat{H}$ is a Hermitian operator, then there exists Eigenfunctions, or special wave functions, Ψ_n, such that

$$\hat{H}\Psi_n = E_n\Psi_n \tag{4}$$

where E_n is purely real. In this case, the time evolution of ψ_n from (2) is

$$\Psi(t) = e^{-i\frac{E_n}{\hbar}t}\Psi_n(t=0) = e^{-i\omega_n t}\Psi_n(t=0) \tag{5}$$

In the above, $E_n = \hbar\omega_n$, or the energy E_n is related to frequency ω_n via the reduced Planck constant $\hbar$.

Scalar variables that are measurable in classical mechanics, such as p and x, are known as observables in quantum mechanics. They are elevated from scalar variables to operators in quantum mechanics, denoted by a "^" symbol here. In classical mechanics, for a one particle system, the Hamiltonian is given by

$$H = T + V = \frac{p^2}{2m} + V \tag{6}$$

The Hamiltonian contains the information from which the equations of motion for the particle can be derived. But in quantum mechanics, this is not sufficient, and H becomes an operator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V} \tag{7}$$

This operator works in tandem with a wavefunction to describe the state of the particle.

The operator acts on a wave function $\Psi(t)$, where in the coordinate x representation, is $\Psi(x.t)$.

When $\Psi(x.t)$ is an Eigenfunction with energy E_n, it can be expressed as

$$\Psi(x.t) = \Psi_n(x)e^{-i\omega_n t} \tag{8}$$

where $E_n = \hbar\omega_n$. The Schrödinger equation for $\psi_n(x)$ then becomes

$$\hat{H}\Psi_n(x) = \left(\frac{\hat{p}^2}{2m} + \hat{V}\right)\Psi(x) = E_n\Psi(x) \tag{9}$$

For simplicity, we consider an electron moving in free space where it has only a constant kinetic energy but not influenced by any potential energy. In other words, there is no force acting on the electron. In this case, $\hat{V} = 0$, and this equation becomes

$$\frac{\hat{p}^2}{2m}\Psi(x) = E_n\Psi(x) \tag{10}$$

It has been observed by de Broglie that the momentum of a particle, such as an electron which behaves like a wave, has a momentum

$$p = \hbar k \tag{11}$$

where $k = 2\pi/\lambda$ is the wave number of the wave function; This motivates that the operator $\hat{p}$ can be expressed by

$$\hat{p} = -i\hbar\frac{d}{dx} \tag{12}$$

in the coordinate space representation. This is chosen so that if an electron is described by a state function $\psi(x) = c_1e^{ikx}$, then $\hat{p}\psi(x) = \hbar k\psi(x)$. The above motivation for the form of the operator $\hat{p}$ is highly heuristic. Equation (10) for a free particle is then

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi_n(x) = E_n\Psi_n(x) \tag{13}$$

Since this is a constant coefficient ordinary differential equation, the solution is of the form

$$\psi_n(x) = e^{\pm ikx} \tag{14}$$

which when used in (13), yields

$$\frac{\hbar^2k^2}{2m} = E_n \tag{15}$$

Namely, the kinetic energy T of the particle is given by

$$T = \frac{\hbar^2 k^2}{2m} \tag{16}$$

where $p = \hbar k$ is in agreement with de Broglie's finding.

In many problems, the operator $\hat{V}$ is a scalar operator in coordinate space representation which is a scalar function of position $V(x)$. This potential traps the particle within it acting as a potential well. In general, the Schrödinger equation for a particle becomes

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x.t) = i\hbar\frac{\partial}{\partial t}\Psi(x.t) \tag{17}$$

For a particular eigenstate with energy E_n as indicated by (8), it becomes

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi_n(x) = E_n\Psi_n(x) \tag{18}$$

The above is an eigenvalue problem with eigenvalue E_n and Eigenfunction $\Psi_n(x)$. These eigenstates are also known as stationary states, because they have a time dependence indicated by (8). Hence, their probability density functions $|\Psi(x.t)|^2$ are time independent.

These Eigenfunctions correspond to trapped modes in the potential well defined by $V(x)$ very much like trapped guided modes in a dielectric waveguide. These modes are usually countable and they can be indexed by the index n.

In the special case of a particle in free space, or the absence of the potential well, the particle or electron is not trapped and it is free to assume any energy or momentum indexed by the continuous variable k. In (15), the index for the energy should rightfully be k and the Eigenfunctions are uncountably infinite. Moreover, the above can be generalized to two and three dimensional cases.

Chapter (3)

Applications of Shrodenger's Equations

Application of Shrodimger Wave Equation

vii. Application of Schrödinger wave Equation

We have now enough knowledge to study some simple solutions of time-independent Schrödinger equation such as:

1. **Electron in free space.**
2. **Electron in infinite potential well.**
3. **Step potential function (The potential step).**
4. **Potential barrier (The Finite Square Well Potential).**
5. **Potential barrier and well.**
6. **Harmonic oscillator.**

1. Electron in free space (Free particle: Continuous states).

- This simplest one-dimensional problem (Electron in free space means no force acting on the electron), it corresponding to $V(x) = 0$ for any value of x.
- We must have $E > V(x)$ to assure the motion of electron.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + (V(x) - E)\psi(x) = 0 \qquad (1\text{-}1)$$

This is above time-independent Schrödinger's wave equation, and since $V(x) = 0$, this equation become

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \quad \text{(free space)} \qquad (1\text{-}2)$$

Or

$$\left(\frac{\partial^2}{\partial x^2} + k^2\right)\psi(x) = 0 \qquad (1\text{-}3)$$

Where $k^2 = 2mE/\hbar^2$. k being the wave number; The most general solution to eq. above is a combination of two linearly independent wave planes $\psi_+ = e^{ikx}$ and $\psi_- = e^{-ikx}$

$$\psi_k(x) = A_+e^{ikx} + A_-e^{-ikx} \qquad (1\text{-}4)$$

Where A_+ and A_- are two arbitrary constants.

$$\because\ \phi(t) = e^{-i\omega t} \text{ and } \Psi(x.t) = \psi(x) \cdot \phi(t) \qquad (1\text{-}5)$$

Then

$$\Psi(x.t) = A_+e^{i(kx-\omega t)} + A_-e^{-i(kx+\omega t)} \qquad (1\text{-}6)$$

Right- going wave Left-going wave

This formula above of the wavefunction represents the stationary state, which can also be written as

$$\Psi(x.t) = A_+ e^{i(kx-\hbar k^2 t/2m)} \quad + \quad A_- e^{-i(kx+\hbar k^2 t/2m)} \qquad (1\text{-}7)$$

Since $\omega = E/\hbar = \hbar k^2/2m$, the first term $\Psi_+(x.t) = A_+ e^{i(kx-\omega t)}$, represents a wave travelling to the right, while the second term $\Psi_-(x.t) = A_- e^{-i(kx+\omega t)}$,represents a wave travelling to the left. The intensities of these waves are given by $|A_+|^2$ and $|A_-|^2$, respectively. We should note that the wave $\Psi_+(x.t)$ and $\Psi_-(x.t)$ are associated, respectively, with a free particle travelling to the right and to the left with well-defined momenta and energy; $p_\pm = \pm\hbar k$, $E_\pm = \hbar^2 k^2/2m$.

We will comment on the physical implications of this in moment. Since there are no boundary conditions, there are no restrictions on k or on E, all vales yield solutions to the equation. Remember the postulate of de Broglie's wave-particle principle:

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

We also have $p = \sqrt{2mE}$ and $E = p^2/2m$

Which implies the consistency of wave-particle principle and wave mechanics in free space (wave mechanics is based on energy quanta and wave particle duality).

The free particle problem is simple to solve mathematically, yet it presents a number of physical subtleties. Let us discuss briefly three of these subtleties.

First, the probability density corresponding to either solutions

$$P_\pm(x.t) = |\Psi_\pm(x.t)|^2 = |A_\pm|^2 \qquad (1\text{-}8)$$

are constant, for they depend neither on x and t. This is due to the complete loss of information about the position and time for a state with definite values of momentum, $p_\pm = \pm\hbar k$, and energy, $E_\pm = \hbar^2 k^2/2m$. This is consequence of Heisenberg's uncertainty principle: when the momentum and energy of a particle are known exactly, $\Delta p = 0$ and $\Delta E = 0$, there must be total uncertainty about its position and time: $\Delta x \to \infty$ and $\Delta t \to \infty$.

Second, an apparent discrepancy between the speed of the wave and the speed of the particle; it is supposed to represent. The speed of the plane waves $\Psi_\pm(x.t)$ is given by

$$\upsilon_{wave} = \frac{\omega}{k} = \frac{E}{\hbar k} = \frac{\hbar^2 k^2/2m}{\hbar k} = \frac{\hbar k}{2m} \qquad (1\text{-}9)$$

On the other hand, the classical speed of the particle is given by

$$\upsilon_{classical} = \frac{p}{m} = \frac{\hbar k}{m} = 2\upsilon_{wave} \qquad (1\text{-}10)$$

This means that the particle travels twice as fast as the wave that represents it.

Third, the wavefunction is not normalizable:

$$\int_{-\infty}^{+\infty} \Psi_{\pm}^{*}(x.t)\Psi_{\pm}(x.t)\,dx = |A_{\pm}|^2 \int_{-\infty}^{+\infty} dx \to \infty \qquad (1\text{-}11)$$

The solution $\Psi_{\pm}(x.t)$ are thus unphysical; physical wavefunctions must be square integrable. The problem can be traced to this; a free particle cannot have sharply defined momenta and energy.

In view of these three subtleties above, the solution of the Schrödinger equation related to this case, that are physically acceptable cannot be planes waves. The answer is provided wave packet

$$\Psi(x.t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \emptyset(k) e^{i(kx-\omega t)} dk. \qquad (1\text{-}12)$$

Where $\emptyset(k)$, the amplitude of the wave packet, is given by the Fourier transform of $\psi(x.0)$ as

$$\emptyset(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x.0) e^{-ikx} dx. \qquad (1\text{-}13)$$

The wave packet solution cures and avoids all the subtleties raised above. First, the momentum, the position and the energy of the particle are no longer known exactly; only probabilistic outcomes are possible. Second, the wave packet (1-12) and the particle travel with the same speed $v_g = p/m$, called the *group* speed or the speed of the whole packet.
Third, the wave packet (1-12) is normalizable. To summarize, a free particle cannot be represented by a single (monochromatic) plane wave; it has to be represented by a wave packet. The physical solutions of the Schrödinger equation are thus given by wave packets, not by stationary solutions.

Q4:-Wave Function for a Free Particle

A free electron has wave function

$$\Psi(x,t) = sin(kx - \omega t) \qquad (1)$$

1. Determine the electron's de Broglie wavelength, momentum, kinetic energy and speed when $k = 50nm^{-1}$.
2. Determine the electron's de Broglie wavelength, momentum, total energy, kinetic energy and speed when $k = 50\ pm^{-1}$.

Solution:-

1. The equations relating the speed v, momentum p, de Broglie wavelength λ, wave number k, kinetic energy E, angular frequency ω and group velocity v_g for a nonrelativistic particle of mass m are:

$$p = mv = \frac{h}{\lambda} = \hbar k \qquad (2)$$

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad (3)$$

$$v_g = \frac{d\omega}{dk} = v \qquad (4)$$

When $k = 50\ nm^{-1}$,

$$\lambda = 126\ \text{pm}, \qquad \text{p} = 9.87\text{KeV}/c \tag{5}$$

And, for an electron ($m = 511\ keV/c^2$),

$$E = 95.2\text{eV}, \qquad \text{v} = 1.93 \times 10^{-2} c \tag{6}$$

2. The equations relating the speed v, momentum p, de Broglie wavelength λ, wave number k, total energy E, kinetic energy K, angular frequency ω and group velocity v_g for a relativistic particle of mass m are:

$$p = \gamma m v = \frac{h}{\lambda} = \hbar k \tag{7}$$

$$E = \gamma mc^2 = mc^2 + K = \sqrt{p^2c^2 + m^2c^4} = \hbar\omega \tag{8}$$

$$v_g = \frac{d\omega}{dk} = v = \frac{pc^2}{E} \tag{9}$$

$$\gamma = \frac{1}{\sqrt{1-\beta^2}} \tag{10}$$

$$\beta = v/c \tag{11}$$

When $k = 50\ pm^{-1}$,

$$\lambda = 126\ \text{fm}, \qquad \text{p} = 9.87\text{MeV}/c \tag{12}$$

And, for an electron ($m = 511\ keV/c^2$),

$$E = 9.88\ \text{MeV}, \quad \text{K} = 9.37\text{MeV} \quad \text{v} = 0.9987\ c \tag{13}$$

Q5:- Potential Energy of a Particle

In a region of space, a particle with mass m and with zero energy has a time-independent wave function

$$\psi(x) = Axe^{-x^2/L^2} \tag{14}$$

Where A and L are constants.

Determine the potential energy U(x) of the particle.

Solution:-

The time-independent Schrödinger equation for the wavefunction $\psi(x)$ of a particle of mass m in a potential $U(x)$ is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = E\psi(x) \tag{15}$$

When a particle with zero energy has wavefunction $\psi(x)$ given by Eq. (14), it follows on substitution into Eq. (15) that

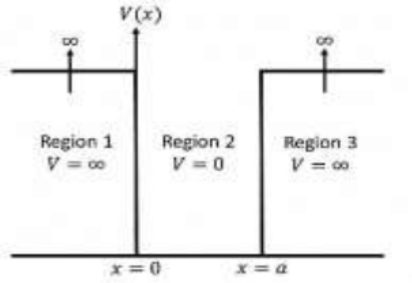
$$U(x) = \frac{2\hbar^2}{mL^4}\left(x^2 - \frac{3L^2}{2}\right) \tag{16}$$

$U(x)$ is a parabola centred at $x = 0$ with $U(x) = \frac{-3\hbar^2}{mL^2}$.

2. Electron in infinite potential well (bound particle)

a. The Asymmetric square well.

Consider a particle of mass m confined to move inside an infinitely deep asymmetric potential well.



$$V(x) = \begin{cases} +\infty & x < 0. \\ 0 & 0 \le x \le a. \\ +\infty & x > a. \end{cases} \qquad (2.1)$$

Classically, the particle remains confined inside the well, moving at constant momentum $p = \pm\sqrt{2mE}$ back and forth as a result of repeated reflection from the walls of the wsell.
Quantum mechanically, we expect this particle to have only bound state solutions and a discrete nondegenerate energy spectrum. Since $V(x)$ is infinite outside the region $0 \le x \le a.$ the wavefunction of the particle must be zero outside the boundary.

Region 1 & 3

$V(x) = \infty$ and $V(x) > E$

⇒ Decaying wave

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}[V(x) - E]\psi(x) = 0$$

Region 2

$V(x) = o$ and $E > V(x)$

⇒ Travelling wave

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

Hence we can look for solutions only inside the well, in the same way that we have learned in "Fundamental physics"

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0. \quad \text{with } k^2 = \frac{2mE}{\hbar^2} \qquad (2\text{-}2)$$

So that, the solution will be

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \Rightarrow \psi(x) = Acos(kx) + Bsin(kx) \qquad (2\text{-}3)$$

Boundary conditions

$\psi(x)$ must continuous (at boundaries and the wavefunction vanishes at the walls).

$$\psi(0) = \psi(a) = 0$$
$$\psi(x = 0^+) = \psi(x = 0^-) = 0 \qquad (2\text{-}4)$$

And

$$\psi(x = a^+) = \psi(x = a^-) = 0 \qquad (2\text{-}5)$$

Since $Acos(k0) = Acos(ka) = 0$

Then $A = 0$

Because $cos(k0) \neq o$ and $cos(ka) \neq 0$

But $Bsin(ka) = 0$

Then $sin(ka) = 0$

Because $B \neq 0$

And $k_n a = n\pi \quad (n = 1.2.3.\cdots)$

This condition above determines the energy

$$E_n = \frac{\hbar^2}{2m}k_n^2 = \frac{\hbar^2\pi^2}{2ma^2}n^2 \quad (n = 1.2.3.\cdots) \qquad (2\text{-}6)$$

The energy is *quantized*; only certain values are permitted. This is expected since the *states* of a particle which is confined to a limited region of space are bounded and the energy spectrum is discrete. This is in sharp contrast to classical physics where the energy of the particle, given by $E = p^2/2m$, takes any value; the classical energy evolves *continuously*. As it can be inferred from (2-6), we should note that the energy between adjacent levels is not constant:

$$E_{n+1} - E_n = 2n + 1 \qquad (2\text{-}7)$$

Which leads

$$\frac{E_{n+1} - E_n}{E_n} = \frac{(n+1)^2 - n^2}{n^2} = \frac{2n+1}{n^2} \qquad (2\text{-}8)$$

In the classical limit $n \to \infty$,

$$\lim_{n\to\infty} \frac{E_{n+1} - E_n}{E_n} = \lim_{n\to\infty} \frac{2n+1}{n^2} = 0 \qquad (2\text{-}9)$$

The levels become so close together as to be practically indistinguishable.
Since $A = 0$ and $k_n = n\pi/a$, then the wavefunction yields $\psi_n(x) = B\sin(n\pi x/a)$, and we can choose the constant B so that $\psi_n(x)$ is normalized (total probability equal one):

$$1 = \int_0^a |\psi_n(x)|^2\, dx = |B|^2 \int_0^a \sin^2(n\pi x/a)\, dx \qquad (2\text{-}10)$$

$$\int_0^a \left(B\sin(kx)\right)^2 dx = 1 \qquad (2\text{-}11)$$

$$\int \sin^2(kx)\, dx = \frac{x}{2} - \frac{\sin 2kx}{4k} \qquad (2\text{-}12)$$

$$\int_0^a \left(B\sin(kx)\right)^2 dx = 1 = B^2 \left(\frac{x}{2} - \frac{\sin 2kx}{4k}\right)\Big|_0^a \qquad (2\text{-}13)$$

($\sin 2kx$ evaluates to 0 at both limits)

$$B = \sqrt{\frac{2}{a}}$$

Hence

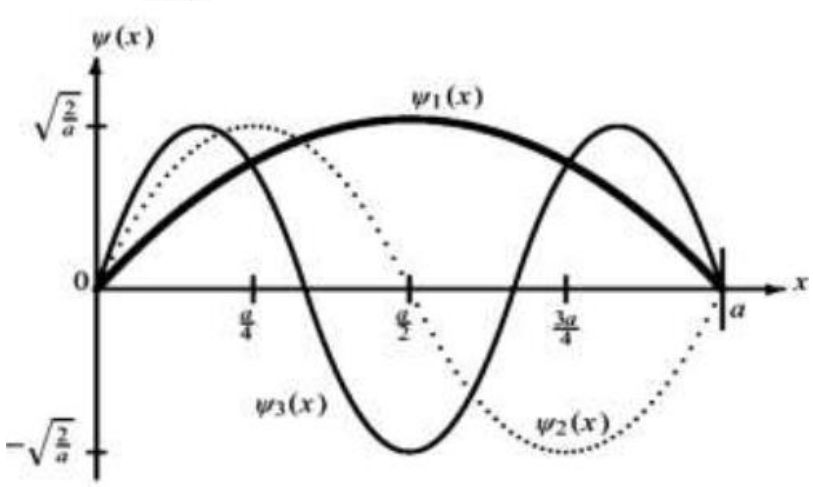
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad (n = 1.2.3.\cdots) \qquad (2\text{-}14)$$

The solution of the time-independent Schrödinger equation has thus given us the energy (2-6) and the wave function (2-14). There is then an infinite sequence of discrete energy levels corresponding to the positive integer values of the *quantum number* n. It is clear that $n = 0$, yields an uninteresting result: $\psi_0(x) = 0$ and $E_o = 0$;later, we will examine in more detail the physical implications of this. So, the lowest energy, or *ground state* energy, corresponds to $n = 1$; it is $E_1 = \hbar^2\pi^2/(2ma^2)$. As will be explained later, this is called the *zero-point energy*, for there exists no state with zero energy. The states corresponding to $n = 2.3.4.\cdots$ are called *excited states*; their energies are given by $E_n = n^2 E_1$. As shown in Figure above, we can see that each function $\psi_n(x)$ has$(n-1)$ nodes, and the functions $\psi_{2n+1}(x)$ are *even* and the functions $\psi_{2n}(x)$ are *odd* with respect to the center of the well;
Note that none of the energy levels is degenerate (there is only one eignfunction for each energy level) and that the wavefunctions corresponding to different energy levels are orthogonal:

$$\int_0^a \psi_m^*(x)\psi_n(x)dx = \delta_{mn} \qquad (2\text{-}15)$$

Since we are dealing with stationary states and since $E_n = n^2 E_1$, the most general solutions of the time-dependent Schrödinger equation are given by

$$\Psi(x.t) = \sum_{n=1}^{\infty} \psi_n(x) e^{-iE_n t/\hbar} = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} sin\left(\frac{n\pi x}{a}\right) e^{-in^2 E_1 t/\hbar} \qquad (2\text{-}16)$$

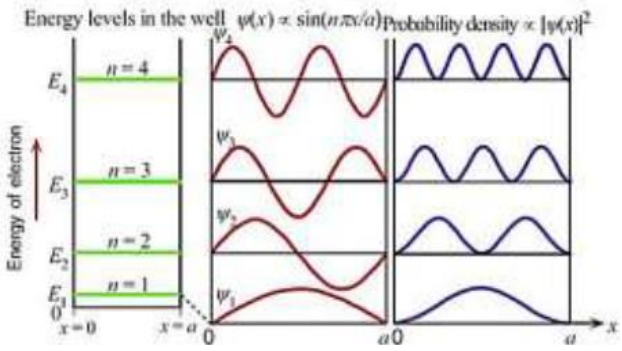


Quantization of energy levels

$$\because k = \sqrt{\frac{2mE}{\hbar^2}}$$

Discrete Wave vector $k = \frac{n\pi}{a}$ ⇒ discrete energy $E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$

Infinite well $E_n \propto n^2$

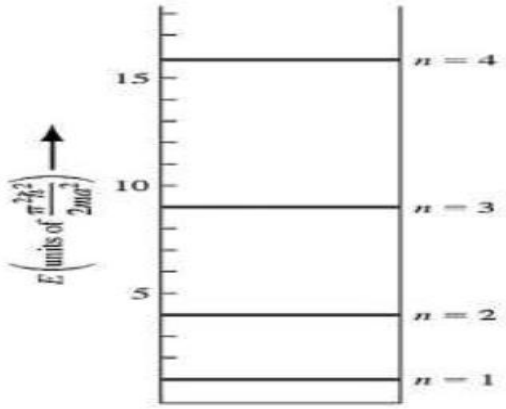


Example: infinite potential well

Infinite potential well width of $5\dot{A}$

$$E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = \frac{n^2(1.054 \times 10^{-34})^2 \pi^2}{2(9.11 \times 10^{-34})(5 \times 10^{-10})^2} = n^2(2.41 \times 10^{-19})J$$
$$= \frac{n^2(2.41 \times 10^{-19})}{1.6 \times 10^{-19}} = n^2(1.51)eV$$

$E_1 = 1.51\ eV$
$E_2 = 6.04\ eV = 4E_1$
$E_3 = 13.59\ eV = 9E_1$
For potential, well, $E_n \propto n^2$



b. The symmetric potential well

In this case, the potential well that previously described, is translated to the left by a distance of $a/2$ to become symmetric

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

First, we would expect the energy spectrum (ii-6) to remain unaffected by this translation, since the Hamiltonian is invariant under spatial translations; as it contains only a kinetic part, it commutes with the particle's momentum, $[\hat{H}.\hat{P}] = 0$. The energy spectrum is discrete and nondegenerate.

Second, earlier in this chapter we saw that for symmetric potentials, $V(-x) = V(x)$, the wave function of bound states must be either even or odd. The wave function corresponding to the potential that described in Eq. above can be written as follows:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\ sin\left[\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right] = \begin{cases} \sqrt{\frac{2}{a}} cos\left(\frac{n\pi}{a}x\right) & (n = 1.3.5.\cdots). \\ \sqrt{\frac{2}{a}} sin\left(\frac{n\pi}{a}x\right) & (n = 2.4.6.\cdots). \end{cases}$$

That is, the wave functions corresponding to odd quantum numbers are symmetric $n = 1.3.5.\cdots$, are symmetric $(-x) = \psi(x)$, and those corresponding to even numbers $n = 2.4.6.\cdots$are antisymmetric, $\psi(-x) \neq \psi(x)$.

3. Harmonic oscillator.

The harmonic oscillator is one of those few problems that are important to all branches of physics. It provides a useful model for a variety of vibrational phenomena that are encountered ,for instance, in classical mechanics, electrodynamics, statistical mechanics, solid state, atomic ,nuclear, and particle physics. In quantum mechanics, it serves as an invaluable tool to illustrate the basic concepts and the formalism.

The paradigm for a classical harmonic oscillator is a mass m attached to a spring of force constant k. The motion is governed by Hooke's law.

$$F = -kx = m\frac{d^2x}{dt^2} \tag{3-1}$$

(as always, we ignore friction), and the solution is

$$x(t) = Asin(\omega t) + Bcos(\omega t) \tag{3-2}$$

Where $\omega \equiv \sqrt{\frac{k}{m}}$ is the (angular) frequency of oscillation. The potential energy is

$$V(x) = \frac{1}{2}kx^2 \tag{3-3}$$

Its graph is a parabola.

Of course, there's no such thing as a perfect simple harmonic oscillator-if you stretch it too far the spring is going to break, and typically **Hook's law** fails long before that point is reached. But practically any potential is *approximately* parabolic, in the neighborhood of a local minimum (Figure below). Formally, if we expand $V(x)$ in a **Taylor series** about the minimum:

$$V(x) = V(x_o) + V'(x_o)(x - x_o) + \frac{1}{2}V''(x_o)(x - x_o)^2 + \cdots \tag{3-4}$$

Subtract $V(x_o)$ [you can add a constant to $V(x_o)$ with impunity, since that doesn't change the force], recognize that $V' = 0$ (since x_o is a minimum), and drop the higher –order terms [which are negligible as long as $(x - x_o)$ stays small], the potential becomes

$$V(x) \cong \frac{1}{2}V''(x_o)(x - x_o)^2 \tag{3-5}$$

Which described simple harmonic oscillation (about the point x_o), with an effective spring constant $k = V''(x_o)$. That's why the simple harmonic oscillator is so important: virtually any oscillatory motion is approximately simple harmonic, as long as the amplitude is small.

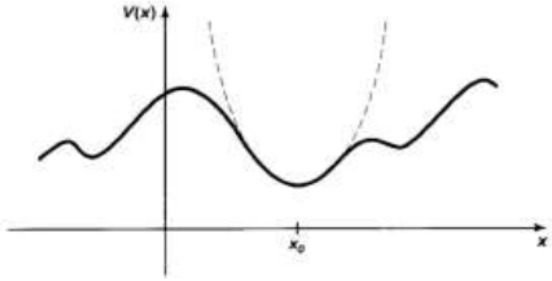


Figure: Parabolic approximation (dashed curve) to an arbitrary potential, in the neighborhood of a local minimum.

The quantum mechanics problem is to solve the Schrödinger equation for the potential

$$V(x) = \frac{1}{2}m\omega^2x^2 \tag{3-6}$$

(it is customary to eliminate the spring constant in favor of the classical frequency, using Equation (6-6). As we have seen, it suffices to solve the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\omega \tag{3-7}$$

In the literature you will find two entirely different approaches to this problem. The first called the *analytic method*, which is a straightforward "brute force" solution to differential equation, using the method of power series expansion; it has the virtue that the same strategy can be applied to many others potentials. The second method is a diabolically clever algebraic technique, using so-called the ladder or algebraic method, does not deal with solving the

Schrödinger equation, but deals instead with operator algebra involving operators known as the *creation* and *annihilation* or ladder operators.

a. Algebraic method

To begin with, let's rewrite Equation (6-7) in a more suggestive form

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2+(m\omega\, x)^2\right]\psi = E\psi \qquad (3\text{-}8)$$

The idea is to factor the term in square brackets. If these were numbers, it would be

$$u^2+v^2=(u-iv)(u+iv)$$

Here, however, it's not quite so simple, because u and v are operators, and operators do not, in general, commute (uv is not the same as vu). Still, this does invite us to take a look at the expressions

$$a_\pm \equiv \frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d}{dx}\pm im\omega\, x\right) \qquad (3\text{-}9)$$

What is their product, a_-a_+ ? Warring: operators can be slippery to work with in the abstract, and you are bound to mike mistake unless you give them a "test function", $f(x)$, to act on. At the end you can throw away the test function, and you'll be left with an equation involving the operators alone. In the present case, we have

$$\begin{aligned}(a_-a_+)f(x) &= \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}-im\omega\, x\right)\left(\frac{\hbar}{i}\frac{d}{dx}+im\omega\, x\right)f(x)\\ &= \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}-im\omega\, x\right)\left(\frac{\hbar}{i}\frac{df}{dx}+im\omega\, xf\right)\\ &= \frac{1}{2m}\left[-\hbar^2\frac{d^2f}{dx^2}+\hbar m\omega\frac{d}{dx}(xf)-m\omega\, x\frac{df}{dx}+(m\omega\, x)^2f\right]\\ &= \tfrac{1}{2m}\left[\left(\tfrac{\hbar}{i}\tfrac{d}{dx}\right)^2+(m\omega\, x)^2+\hbar m\omega\right]f(x)\end{aligned} \qquad (3\text{-}10)$$

[I used $d(xf)/dx = x(df/dx)+f$ in the last step]. Discarding the test function, we conclude that

$$a_-a_+ = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2+(m\omega\, x)^2\right]+\frac{1}{2}\hbar\omega \qquad (3\text{-}11)$$

Evidently, Equation (vi-8) does not factor perfectly – there's an extra term $(1/2)\hbar\omega$. However, if we pull this over to the other side, the Schrödinger equation becomes

$$\left(a_-a_+-\frac{1}{2}\hbar\omega\right)\psi = E \qquad (3\text{-}12)$$

Notice that the ordering of the factors a_+ and a_- is important here, the same argument with a_+ on the left yields

$$a_+a_- = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2-(m\omega\, x)^2\right]-\frac{1}{2}\hbar\omega \qquad (3\text{-}13)$$

Thus

$$a_-a_+ - a_+a_- = \hbar\omega \qquad (3\text{-}14)$$

And the Schrödinger equation can also be written

$$\left(a_+a_-+\frac{1}{2}\hbar\omega\right)\psi = E\psi \qquad (3\text{-}15)$$

Now, here comes the crucial step: I claim that if ψ; satisfies the Schrödinger equation, with energy E, then $a_+\psi$ satisfies the Schrödinger equation with energy (E +hw). Proof:

$$\left(a_+a_- + \frac{1}{2}\hbar\omega\right)(a_+\psi) = \left(a_+a_-a_+ + \frac{1}{2}\hbar\omega\, a_+\right)\psi$$
$$= a_+\left(a_-a_+ + \frac{1}{2}\hbar\omega\right)\psi = a_+\left[\left(a_-a_+ - \frac{1}{2}\hbar\omega\right)\psi + \hbar\omega\psi\right]$$
$$= a_+(E\psi + \hbar\omega\psi) = (E + \hbar\omega)(a_+\psi).\, QED$$

Notice that whereas the ordering of a_+ and a_- does matter, the ordering of $a_\pm$ and any constants (such as $\hbar$, ω, and E) does not.] By the same token, $a_-\psi$ is a solution with energy$(E - \hbar\omega)$:

$$\left(a_-a_+ - \frac{1}{2}\hbar\omega\right)(a_-\psi) = a_-\left(a_+a_- - \frac{1}{2}\hbar\omega\right)\psi$$
$$= a_-\left[\left(a_+a_- + \frac{1}{2}\hbar\omega\right)\psi - \hbar\omega\psi\right] = a_-(E\psi - \hbar\omega\psi)$$
$$= (E - \hbar\omega)(a_-\psi).\, QED$$

Here, then, is a wonderful machine for grinding out new solutions, with higher and lower energies—if we can just find one solution, to get started! We call $a_\pm$ ladder operators, because they allow us to climb up and down in energy; a_+ is called *the raising operator*, and a_- *the lowering operator*. The "ladder" of states is illustrated in Figure below.

But wait! What if I apply the lowering operator repeatedly? Eventually I'm going to reach a state with energy less than zero, which (according to the general theorem) does not exist! At some point the machine must fail. How can that happen? We know that $a_-\psi$ is a new solution to the Schrödinger equation, but there is no guarantee that it will be normalizable—it might be zero, or its square integral might be infinite. Conclusion: There must occur a "lowest rung" (let's call it ψ_o) such that

$$a_-\psi = 0 \qquad (3\text{-}16)$$

That is to say

$$\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d\psi_o}{dx} - im\omega\, x\, \psi_o\right) = 0$$

Or

$$\frac{d\psi_o}{dx} = -\frac{m\omega}{\hbar}x\,\psi_o$$

This differential equation for ψ_o is easy to solve:

$$\int \frac{d\psi_o}{\psi_o} = -\frac{m\omega}{\hbar}\int x dx \quad \Rightarrow \quad ln\psi_o = -\frac{m\omega}{2\hbar}x^2 + constant,$$

So

$$\psi_o(x) = A_o e^{-\frac{m\omega}{2\hbar}x^2}. \qquad (3\text{-}17)$$

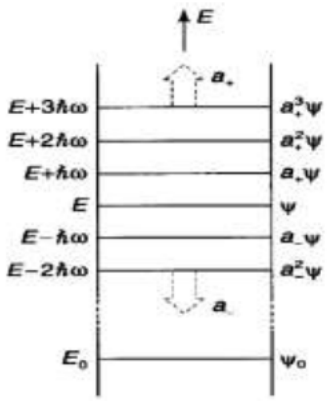


Figure: the ladder of stationary states for the simple harmonic oscillator.

To determine the energy of this state, we plug it into the Schrödinger equation {in the form of Equation (6-15}, $\left(a_+a_- + \frac{1}{2}\hbar\omega\right)\psi_o = E_o\psi_o$, and exploit the fact that $a_-\psi = 0$. Evidently

$$E_o = \frac{1}{2}\hbar\omega \tag{3-18}$$

With our foot now securely planted on the bottom rung" (the ground state of the quantum oscillator), we simply apply the raising Operator to generate the excited states":

$$\psi_n(x) = A_n(a_+)^n e^{-\frac{m\omega}{2\hbar}x^2}, \qquad with\ E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{3-19}$$

(This method does not immediately determine the normalization factor A_n; For example,

$$\psi_1(x) = A_1 a_+ e^{-\frac{m\omega}{2\hbar}x^2} = A_1\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d}{dx} - im\omega\, x\right)e^{-\frac{m\omega}{2\hbar}x^2}$$

$$= \frac{A_1}{\sqrt{2m}}\left(\frac{\hbar}{i}\left(-\frac{m\omega}{\hbar}x\right)e^{-\frac{m\omega}{2\hbar}x^2} + im\omega\, x e^{-\frac{m\omega}{2\hbar}x^2}\right)$$

Which simplify to

$$\psi_1(x) = \left(iA_1\omega\sqrt{2m}\right)xe^{-\frac{m\omega}{2\hbar}x^2} \tag{3-20}$$

I wouldn't want to calculate ψ_{50} in this way, but never mind: We have found all the allowed energies, and in principle we have determined the stationary states—the rest is just computation.

a. Analytical Method

We return now to the Schrödinger equation for the harmonic oscillator (Equation 3-7):

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

Things look a little cleaner if we introduce the dimensionless variable

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x \tag{3-21}$$

In term of ξ, the Schrödinger reads

$$\frac{d^2\psi}{dx^2} = (\xi^2 - K)\psi \tag{3-22}$$

Where K is the energy, in units of $(1/2)\hbar\omega$:

$$K \equiv \frac{2E}{\hbar\omega} \tag{3-23}$$

Our problem is to solve Equation 3-22, and in the process obtain the "allowed" values of K (and hence of E).

To begin with, note that at very large ξ (which is to say, at very large x), ξ^2completely dominates over the constant K, so in this regime

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi \tag{3-24}$$

which has the approximate solution (check it!)

$$\psi(\xi) \approx Ae^{-\xi^2/2} + Be^{+\xi^2/2} \tag{3-25}$$

The B term is clearly not normalizable (it blows up as $|x| \to \infty$); the physically acceptable solutions, then, have the asymptotic for

$$\psi(\xi) \approx ()e^{-\xi^2/2}, \quad \text{at large } \xi \tag{3-26}$$

This suggests that we "peel off ' the exponential part,

$$\psi(\xi) = h(\xi)e^{-\xi^2/2}, \tag{3-27}$$

in hopes that what remains $[h(\xi)]$ has a simpler functional form than $\psi(\xi)$ itself. Differentiating Equation 3-26, we have

$$\frac{d\psi}{d\xi} = \left(\frac{dh}{d\xi} - \xi h\right)e^{-\xi^2/2}$$

And

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)\right)e^{-\xi^2/2}$$

So the Schrödinger equation (Equation 3-21) becomes

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0, \tag{3-28}$$

I propose to look for a solution to Equation 6-28 in the form of a power series in ξ:

$$h(\xi) = a_o + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j\xi^j, \tag{3-29}$$

Differentiating the series term by term,

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 \ldots = \sum_{j=0}^{\infty} j a_j\xi^{j-1}, \tag{3-30}$$

And

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2\cdot 3a_3\xi + 3\cdot 4a_4\xi^2 + \cdots = \sum_{j=0}^{\infty}(j+1)(j+2)a_{j+2}\xi^j, \tag{3-31}$$

Putting these into Equation 3-27, we find

$$\sum_{j=0}^{\infty}[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j]\xi^j = 0\ , \tag{3-32}$$

It follows (from the uniqueness of power series expansions") that the coefficient of *each power* of ξ must vanish

$$(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j = 0$$

And hence that

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j, \tag{3-33}$$

This **recursion formula** is entirely equivalent to the Schrödinger equation itself. Given a_o it enables us (in principle) to generate $a_2, a_4, a_6, \ldots$ and given a_1 it generates $a_3, a_5, a_7, \ldots$. Let us write

$$h(\xi) = h_{even}(\xi) + h_{odd}(\xi) \tag{3-34}$$

Where

$$h_{even}(\xi) = a_o + a_2\xi^2 + a_4\xi^4 + \cdots$$

is an even function of ξ (since it involves only even powers), built on a_o, and

$$h_{odd}(\xi) = a_1\xi + a_3\xi^3 + a_5\xi^5 + \cdots$$

is an odd function, built on a_1. Thus Equation vi-31 determines $h(\xi)$ in terms arbitrary constants (a_o and a_1)—which is just what we would expect, for a second order differential equation.

However, not all the solutions so obtained are normalizable. For at very large j, the recursion formula becomes (approximately)

$$a_{j+2} \approx \frac{2}{j} a_j,$$

With the (approximate) solution

$$a_j \approx \frac{C}{(j/2)!},$$

For some constant C, and this yields (at large ξ, where the higher powers dominate)

$$h(\xi) \approx C \sum \frac{1}{(j/2)!} \xi^j \approx C \sum \frac{1}{k!} \xi^{2k} \approx C e^{\xi^2}$$

Now, if h goes like $exp(\xi^2)$, then ψ (remember ψ?——that's what we're trying to calculate) goes like $\exp(\xi^2/2)$, (Equation vi-27), which is precisely the asymptotic behavior we don 't want." There is only one way to wiggle out of this: For normalizable solutions the power series must terminate. There must occur some "highest" j (call it n) such that the recursion formula spits out $a_{n+2} = 0$ (this will truncate either the series h_{even} or the series h_{odd}; the other one must be zero from the start). For physically acceptable solutions, then, we must have

$$K = 2n + 1,$$

for some positive integer n , which is to say (referring to Equation 3-23) that the energy must be of the form

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad for\ n = 0,1,2, ... \qquad (3\text{-}35)$$

Thus we recover, by a completely different method, the fundamental quantization condition we found algebraically in Equation 3-19.

For the allowed values of K, the recursion formula reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j \qquad (3\text{-}36)$$

If $n = 0$, there is only one term in the series (we must pick a_1 to kill h_{odd}, and $j = 0$ in Equation. 3-36 yields $a_1 = 0$):

$$h_0(\xi) = a_0,$$

And hence

$$\psi_0(\xi) = a_0 e^{-\xi^2/2}$$

(which reproduces Equation 3-17). For $n = 0$ we pick $a_0 = 0$, and Equation 6-36 with $j = 0$ yields $a_3 = 0$, so

$$h_1(\xi) = a_1 \xi,$$

And hence

$$\psi_1(\xi) = a_1 \xi e^{-\xi^2/2}$$

(confirming Equation 3-20). For $n = 2$, $j = 0$yields $a_2 = -2a_0$, andj $j = 2$ gives $a_4 = 0$, so

$$h_2(\xi) = a_o(1 - 2\xi^2),$$

And

$$\psi_2(\xi) = a_o(1 - 2\xi^2)e^{-\xi^2/2}$$

and so on.

In general, $h_n(\xi)$ will be a polynomial of degree n in ξ, involving even powers only, if n is an even integer, and odd powers only, if n is an odd integer. Apart from the overall factor (a_o or a_1) they are the so-called Hermite polynomials, $H_n(\xi)$.

The Hermite polynomials is:

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{dx^n} e^{\xi^{-2}}$$

The first few of them are listed in Table below. By tradition, the arbitrary multiplicative factor is chosen so that the coefficient of the highest power of 'ξ is 2^n". With this convention, the normalized stationary states for the harmonic oscillator are

$$\psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \qquad (3\text{-}37)$$

They are identical (of course) to the ones we obtained algebraically in Equation 3-19.
In Figure below a I have plotted $\psi_n(x)$ for the first few n's.
The quantum oscillator is strikingly different from its classical counterpart—not only are the energies quantized, but the position distributions have some bizarre features. For instance, the probability of finding the particle outside the classically allowed range (that is, with x greater than the classical amplitude for the energy in question) is not zero, and in all odd states the probability of

Table: The first few Hermite polynomials, $H_n(\xi)$.

$H_o = 1,$	For $n = 0,$
$H_1 = 2x,$	For $n = 1,$
$H_2 = 4x^2 - 2,$	For $n = 2,$
$H_3 = 8x^3 - 12x,$	For $n = 3,$
$H_4 = 16x^4 - 48x^2 + 12,$	For $n = 4,$
$H_5 = 32x^5 - 160x^3 + 120x,$	For $n = 5,$

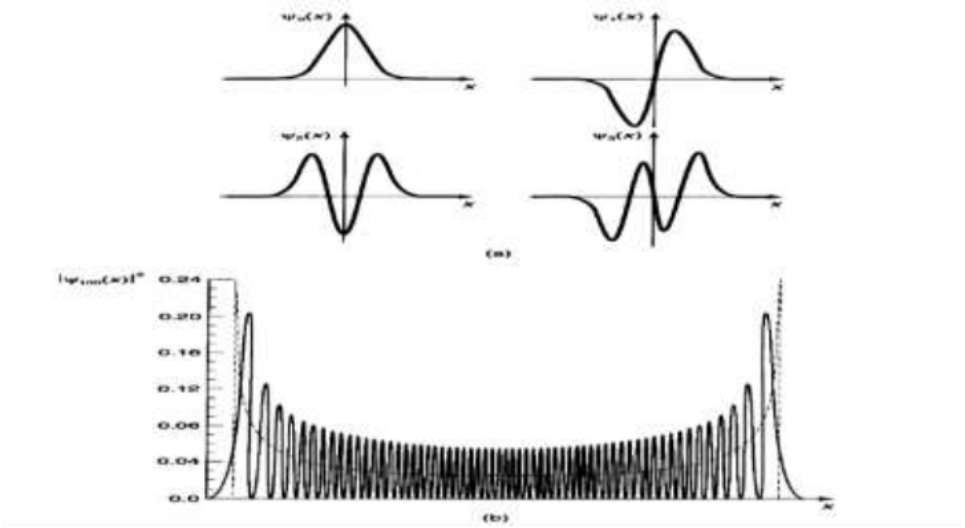


Figure: (a) The first four stationary states of the harmonic oscillator.
(b) Graph of $|\psi_1(x)|^2$, with the classical distribution (dashed curve) superimposed.

finding the particle at the center of the potential well is zero. Only at relatively large n do we begin to see some resemblance to the classical case. In Figure above-b I have superimposed the classical position distribution on the quantum one (for $n = 100$); if you smoothed out the bumps in the latter, the two would fit pretty well (however, in the classical case we are talking about the distribution of positions over *time* for *one* oscillator, whereas in the quantum case we are talking about the distribution over an ensemble of identically-prepared systems).

Q6: The dynamics of a particle moving one-dimensionally in a potential $V(x)$ is governed by the Hamiltonian $H_0 = p^2/2m + V(x)$, where $p = -i\hbar d/dx$ is the momentum operator. Let E_n^0, $n = 1,2,3,\ldots$, be the eigenvalues H_0 . Now consider a new Hamiltonian $H = H_0 + \lambda p/m$, where λ is a given parameter. Given A, m and E_n^0,), find the eigenvalues of H.

Solution:-
The new Hamiltonian is

$$H = H_0 + \lambda p/m = p^2/2m + \lambda p/m + V(x),$$
$$= (p+\lambda)^2/2m + V(x) - \lambda^2/2m,$$

Or

$$H' = \frac{p'^2}{2m} + V(x),$$

Where $H' = H + \frac{\lambda^2}{2m}, p' = p + \lambda,$
The eigenfunctions and eigenvalues of H' are respectively E_n^0 and ψ_n^0.
AS the wave number is $k' = \frac{p'}{\hbar} = \frac{1}{\hbar}(p+\lambda)$,the new eigenfunction are

$$\psi = \psi^0 e^{-\lambda x/\hbar}$$

and the corresponding eigenvalues are

$$E_n = E_n^0 - \lambda^2/2m.$$

Q7: Use the uncertainty principle to obtain the ground state energy of a linear Oscillator.

Solution:-

$$\Delta x \Delta p \sim \hbar/2$$
$$p = \frac{\hbar}{2x}$$
$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$
$$E = \frac{\hbar^2}{8mx^2} + \frac{1}{2}m\omega^2 x^2$$

The ground state energy is obtained by setting $\frac{\partial E}{\partial x} = 0$

$$\frac{\partial E}{\partial x} = -\frac{\hbar^2}{4mx^3} + m\omega^2 x = 0$$

Whence $x^2 = \frac{\hbar}{2m\omega}$

$$\therefore E = 1/4\hbar\omega + 1/4\hbar\omega = \frac{1}{2}\hbar\omega$$

Q8: Derive the probability distribution for a classical simple harmonic oscillator.

Solution:-
One can expect the probability of finding the particle of mass m at distance x from the equilibrium position to be inversely proportional to the velocity

$P(x) = \frac{A}{v}$ (1)

where A =normalization constant. The equation for S.H.O. is

$\frac{d^2x}{dt^2} + \omega^2 x = 0$

which has the solution

$x = a \sin \omega t;\ (at\ t = 0, x = 0)$

where a is the amplitude.

$v = \frac{dx}{dt} = \omega\sqrt{a^2 - x^2}$ (2)

Using (2) in (1)

$P(x) = \frac{A}{\omega\sqrt{a^2-x^2}}$ (3)

We can find the normalization constant A.

$\int P(x)dx = \int_{-a}^{a} \frac{Adx}{\omega\sqrt{a^2-x^2}} = \frac{\pi A}{\omega}$=1

Therefore,

$A = \frac{\omega}{\pi}$ (4)

Using (4) in (3), the normalized distribution is

$P(x) = \frac{1}{\pi\sqrt{a^2-x^2}}$ (5)

Q9: Show that the wavefunction $\psi_o(x) = A\, exp(-x^2/2a^2)$ is a solution to the time- independent Schrodinger equation for a simple harmonic oscillator (SHO) potential.

$$\left(-\frac{\hbar^2}{2m}\right)\frac{d^2\psi}{dx^2} + \left(\frac{1}{2}\right) m\omega_o x^2 \psi = E\,\psi$$

with energy $E_o = \left(\frac{1}{2}\right)\hbar\omega_o$, and determine a in terms of m and ω_o.

The corresponding dimensionless form of this equation is

$-\frac{d^2\psi}{dR^2} + R^2\psi = \varepsilon E$

where $R = x/a$ and $\varepsilon = E/E_o$.

Show that putting $\psi(R) = AH(R)exp(-R^2/2)$ into this equation leads to Hermite's equation

$-\frac{d^2H}{dR^2} - 2R\left(\frac{dH}{dR}\right) + (\varepsilon - 1)H = 0$

$H(R)$ is a polynomial of order n of the form $a_n R_n + a_n - 2\, R_n - 2 + a_n - 4\, R_n - 4 + \ldots$

Deduce that ε is a simple function of n and that the energy levels are equally spaced.

Solution:-

By substituting $\psi(R) = AH(R)\, exp\,(-R^2/2)$ in the dimensionless form of the equation and simplifying we easily get the Hermite's equation.

The problem is solved by the series method

$H = \Sigma H_n(R) = \Sigma_{n=0,2,4} a_n\, R_n$

$\frac{dH}{dR} = a_n n R^{n-1}$

$\frac{d^2H}{dR^2} = \sum n(n-1)\, a_n R^{n-2}$

$\Sigma n(n-1)a_n R^{n-2} - 2\Sigma a_n n R^n + (\varepsilon - 1)\Sigma a_n R^n = 0$

Equating equal power of R_n

$a_{n+2} = \frac{[2n - (\varepsilon - 1)]a_n}{(n+1)(n+2)}$

If the series is to terminate for some value of n then
$2n-(\varepsilon-1)=0$ becuase $a_n=0$. This gives $\varepsilon=2n+1$
Thus ε is a simple function of n
$E=\varepsilon E_o=(2n+1)1/2\hbar\omega, n=0,2,4,\ldots$
$=1/2\hbar\omega, 3\hbar\omega/2, 5\hbar\omega/2,\ldots$
Thus energy levels are equally spaced.

Q10: Show that for a simple harmonic oscillator in the ground state the probability for finding the particle in the classical forbidden region is approximately 16%.

Solution:-

$$u_o=\left[\frac{\alpha}{\sqrt{\pi}}\right]e^{-\zeta^2/2}H_o(\zeta);\zeta=\alpha x$$

$$P=1-\int_{-a}^{a}|u_o|^2\,dx=1-2\int_0^a\left(\alpha/\sqrt{\pi}\right)^2e^{-\zeta^2/2}\,dx=1-\frac{2}{\sqrt{\pi}}\int_0^{a\alpha}e^{-\zeta^2/2}d\zeta$$

$$E_o=1/2\,ka^2=\frac{\hbar\omega}{2}(n=0)$$

Therefore $a^2=\frac{\hbar\omega}{k}=\left(\frac{\hbar}{k}\right)\left(\frac{k}{m}\right)^{1/2}=\frac{\hbar}{\sqrt{km}}=\frac{1}{\alpha^2}$

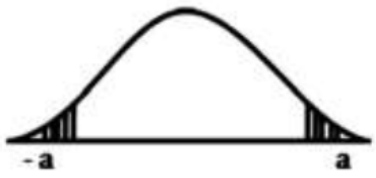
Therefore $\alpha^2a^2=1$ or $\alpha a=1$

$$P=1-\frac{2}{\sqrt{\pi}}\int_0^1e^{-\zeta^2/2}d\zeta=1-\frac{2}{\sqrt{\pi}}\int_0^1\left[1-\zeta^2+\frac{\zeta^4}{2!}-\frac{\zeta^6}{3!}+\frac{\zeta^8}{4!}-\cdots\right]d\zeta$$

$$=1-\frac{2}{\sqrt{\pi}}\left[1-\frac{1}{3}+\frac{1}{10}-\frac{1}{42}+\frac{1}{418}-\cdots\right]\approx 0.16$$

Therefore, $p\approx 16\%$.

Fig. Probability of the particle found outside the classical limits is shown shaded.



Schrödinger Equation in 3D Cartesian Coordinates:

- The stationary Schrodinger equation in three dimensions is a partial differential equation involving three coordinates per particle. The mathematical complexity behind such an equation can be intractable by analytical means. However, there are certain high-symmetry cases when it is possible to separate variables in some convenient coordinate system and reduce the Schrodinger equation to one-dimensional problems.

- The simplest example of variable separation is a particle in infinitely deep three dimensional quantum well. Let the potential $V(x,y,z)$ be zero inside a block with edges a_1, a_2, a_3 and infinite outside:

$$V(\mathbf{r}) = \left\{ \begin{array}{ccc} 0 & , & 0<x<a_1 \ \wedge \ 0<y<a_2 \ \wedge \ 0<z<a_3 \\ \infty & , & \text{otherwise} \end{array} \right\}$$

  We immediately note that this function can be written as a sum of three one-dimensional functions:

$$V(\mathbf{r}) = V_1(x) + V_2(y) + V_3(z)$$

$$V_i(x_i) = \left\{ \begin{array}{ccc} 0 & , & 0<x_i<a_i \\ \infty & , & \text{otherwise} \end{array} \right\}$$

- The Schrodinger equation

$$-\frac{\hbar^2\nabla^2}{2m}\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

  can be expressed as a sum involving individual coordinates:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(\mathbf{r})}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2\psi(\mathbf{r})}{\partial y^2} - \frac{\hbar^2}{2m}\frac{\partial^2\psi(\mathbf{r})}{\partial z^2} + V_1(x)\psi(\mathbf{r}) + V_2(y)\psi(\mathbf{r}) + V_3(z)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

- Whenever the operator acting on the unknown function can be expressed as a sum of operators involving individual coordinates, the solution for the function has the form of a product:

$$\psi(\mathbf{r}) = \psi_1(x)\psi_2(y)\psi_3(z)$$

  Now, the one-variable functions ψ_1, ψ_2 and ψ_3 are unknown. We substitute $\psi(\mathbf{r})$ in the Schrodinger equation and note that the derivative with respect to x acts only on ψ_1, etc.:

$$\begin{aligned} \left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi_1(x)}{\partial x^2} + V_1(x)\psi_1(x)\right]\psi_2(y)\psi_3(z) \quad &+ \\ \left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi_2(y)}{\partial y^2} + V_2(y)\psi_2(y)\right]\psi_3(z)\psi_1(x) \quad &+ \\ \left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi_3(z)}{\partial z^2} + V_3(z)\psi_3(z)\right]\psi_1(x)\psi_2(y) \quad &= \quad (E_1+E_2+E_3)\psi_1(x)\psi_2(y)\psi_3(z) \end{aligned}$$

  We have also expressed the total energy E as a sum of contributions from individual dimensions, $E = E_1 + E_2 + E_3$.

- Consider any point $\mathbf{r}$ at which $\psi(\mathbf{r}) \neq 0$. Divide the whole equation by $\psi(\mathbf{r}) = \psi_1(x)\psi_2(y)\psi_3(z)$:

$$\begin{aligned}
&\frac{1}{\psi_1(x)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi_1(x)}{\partial x^2} + V_1(x)\psi_1(x)\right] \quad + \\
&\frac{1}{\psi_2(y)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi_2(y)}{\partial y^2} + V_2(y)\psi_2(y)\right] \quad + \\
&\frac{1}{\psi_3(z)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi_3(z)}{\partial z^2} + V_3(z)\psi_3(z)\right] \quad = \quad E_1 + E_2 + E_3
\end{aligned}$$

Each term on the left-hand side depends on only one coordinate and hence is completely independent from other terms. The only way to satisfy this equation for any combination of (x, y, z) is to require that three one-dimensional equations be satisfied:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_1(x)}{\partial x^2} + V_1(x)\psi_1(x) = E_1\psi_1(x)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_2(y)}{\partial y} + V_2(y)\psi_2(y) = E_2\psi_2(y)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_3(z)}{\partial z^2} + V_3(z)\psi_3(z) = E_3\psi_3(z)$$

One can now substitute these expressions into the full 3D Schrodinger equation and see that they solve it even at the points $\mathbf{r}$ where $\psi(\mathbf{r}) = 0$. Therefore, the solution of the 3D Schrodinger equation is obtained by multiplying the solutions of the three 1D Schrodinger equations.

- Now, in each dimension we have a simple one-dimensional infinitely deep quantum well problem, which we solved before:

$$E_i = \frac{\pi^2\hbar^2}{2ma_i^2}n_i^2$$

$$\psi_i(x_i) = \sqrt{\frac{2}{a_i}}\sin\left(\frac{\pi n_i}{a_i}x_i\right)$$

- The full 3D solutions are characterized by three positive integer quantum numbers, (n_x, n_y, n_z), one per dimension. The total energy is

$$E = E_1 + E_2 + E_3 = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2}\right)$$

and the full wavefunction is:

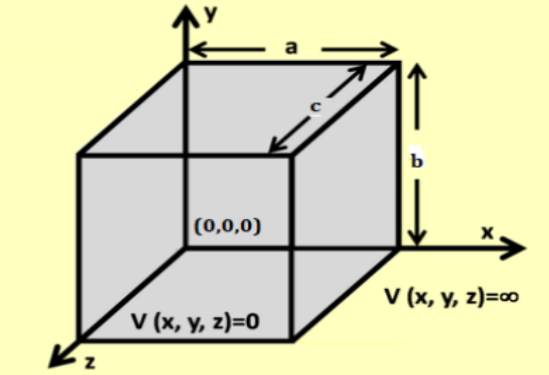
$$\psi(\mathbf{r}) = \psi_1(x)\psi_2(y)\psi_3(z) = \sqrt{\frac{8}{V}}\sin\left(\frac{\pi n_x}{a_x}x\right)\sin\left(\frac{\pi n_y}{a_y}y\right)\sin\left(\frac{\pi n_z}{a_z}z\right)$$

where $V = a_x a_y a_z$ is the volume of the quantum well.

Particle in a 3D Box

A real box has three dimensions. Consider a particle which can move freely with in rectangular box of dimensions a × b × c with impenetrable walls. The potential can be written mathematically as;

$$V = \begin{cases} 0 & \text{Inside} \\ \infty & \text{At surfaces and outside} \end{cases}$$



Since the wavefunction ψ should be well behaved, so, it must vanish everywhere outside the box. By the continuity requirement, the wavefunction must also vanish in the six surfaces of the box. Orienting the box so its edges are parallel to the cartesian axes, with one corner at (0,0,0), the following boundary conditions must be satisfied:

ψ(x,y, z) = 0 when x = 0, x = a, y = 0, y = b, z = 0 or z = c

Inside the box, where the potential energy is everywhere zero, the Hamiltonian is simply the three-dimensional kinetic energy operator and the Schrodinger equation reads

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = E(x,y,z) \qquad (1)$$

Since we can write ψ(x,y, z) = X(x)Y(y)Z(z), with condition X(x) is independent of y and z coordinates. Also, Y(y) and Z(z) are only functions of y and z, respectively. The boundary conditions are

X(0) = X(a) = 0, Y (0) = Y (b) = 0, Z(0) = Z(c) = 0 (2)

So, on substituting (x,y, z) = X(x)Y(y)Z(z) into Schrodinger equation we obtain

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + \frac{2mE}{\hbar^2} = 0 \qquad (3)$$

Each of the first three terms depends on one variable only, independent of the other two. We can write it as;

$$\frac{X''(x)}{X(x)} = -\left[\frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + \frac{2mE}{\hbar^2}\right]$$

Now on left hand side (LHS) we have only function of x, while right hand side (RHS) contains functions of y and z. This is possible only if each term separately equals a constant, say, $-\alpha^2$. So,

$$\frac{X''(x)}{X(x)} = -\left[\frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} + \frac{2mE}{\hbar^2}\right] = -\alpha^2 .$$

$$\Rightarrow \frac{X''(x)}{X(x)} = -\alpha^2$$

That implies $\left[\frac{Y''(y)}{Y(y)}+\frac{Z''(z)}{Z(z)}+\frac{2mE}{\hbar^2}\right]=\alpha^2$ which can be transformed into $\frac{Y''(y)}{Y(y)}=\alpha^2-\left[\frac{Z''(z)}{Z(z)}+\frac{2mE}{\hbar^2}\right]$; Using similar argument as above both sides of eqution should be equal to a constant, say, $-\beta^2$;

Therefore, $\frac{Y''(y)}{Y(y)}=\alpha^2-\left[\frac{Z''(z)}{Z(z)}+\frac{2mE}{\hbar^2}\right]=-\beta^2$

$$\Rightarrow \frac{Y''(y)}{Y(y)}=-\beta^2 \qquad (5)$$

And

$$\alpha^2-\left[\frac{Z''(z)}{Z(z)}+\frac{2mE}{\hbar^2}\right]=-\beta^2$$

$$\Rightarrow \frac{Z''(z)}{Z(z)}=\alpha^2+\beta^2-\frac{2mE}{\hbar^2}$$

Now, LHS of above equation is just a constant so we can write it as a $\frac{Z''(z)}{Z(z)}=-\gamma^2$ (6)

Thereby we have transformed a single Schrodinger equation (1) into three ordinary differential equations

$X''+\alpha^2X=0; Y''+\beta^2Y=0$ and $Z''+\gamma^2Z=0$

The constants α, β and γ are related by

$$\frac{2mE}{\hbar^2}=\alpha^2+\beta^2+\gamma^2 \qquad (7)$$

Each of the equations (4, 5 and 6) with its associated boundary conditions in (2) is equivalent to the one-dimensional problem. The normalized solutions X(x), Y (y), Z(z) can therefore be written down in complete analogy with one dimensional box

$$X_{n1}(x) = \left(\frac{2}{a}\right)^{1/2} Sin\frac{n_1\pi x}{a}; \qquad n_1 = 1,2,3..... \tag{8}$$

$$Y_{n2}(x) = \left(\frac{2}{a}\right)^{1/2} Sin\frac{n_2\pi y}{b}; \qquad n_2 = 1,2,3.... \tag{9}.$$

$$Z_{n3}(x) = \left(\frac{2}{a}\right)^{1/2} Sin\frac{n_2\pi z}{c}; \qquad n_3 = 1,2,3..... \tag{10}$$

The constants in Eq (7) are given by

$$\alpha = \frac{n_1\pi}{a};\ \beta = \frac{n_2\pi}{b} \text{ and } \gamma = \frac{n_3\pi}{c}$$

and the allowed energy levels are therefore

$$E_{n_1,n_2,n_3} = \frac{h^2}{8m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\right), \qquad n_1, n_2, n_3 = 1, 2... \tag{11}$$

Three quantum numbers are required to specify the state of this three dimensional system. The corresponding eigen-functions are

$$\psi_{n_1,n_2,n_3}(x,y,z) = \left(\frac{8}{V}\right)^{1/2} Sin\frac{n_1\pi x}{a} Sin\frac{n_2\pi x}{b} Sin\frac{n_3\pi x}{c} \tag{12}$$

where V = abc, the volume of the box. These eigen-functions form an ortho-normal set such that

$$\int_0^a\int_0^b\int_0^c \psi_{n'_1,n'_2,n'_3}(x,y,z)\psi_{n_1,n_2,n_3}(x,y,z)dxdydz = \delta_{n'_1,n_1}\delta_{n'_2,n_2}\delta_{n'_3,n_3}$$

Note that two eigen-functions will be orthogonal unless all three quantum numbers match.

When the box has the symmetry of a cube, with a = b = c, the energy formula (11) simplifies to

$$E_{n_1,n_2,n_3} = \frac{h^2}{8ma^2}\left(n_1^2 + n_2^2 + n_3^2\right), \qquad n_1, n_2, n_3 = 1, 2... \tag{13}$$

Quantum systems with symmetry generally exhibit degeneracy in their energy levels. This means that there can exist distinct eigenfunctions which share the same eigenvalue. An eigenvalue which corresponds to a unique eigenfunction is termed nondegenerate while one which belongs to n different eigenfunctions is termed n-fold degenerate. As an example, we enumerate the first few levels for a cubic box, with E_{n_1,n_2,n_3} expressed in units in units of $h^2/8ma^2$.

$$E_{1,1,1} = 3 \text{ (nondegenerate)}$$
$$E_{1,1,2} = E_{1,2,1} = E_{2,1,1} = 6 \text{ (3-fold degenerate)}$$
$$E_{1,2,2} = E_{2,1,2} = E_{2,2,1} = 9 \text{ (3-fold degenerate)}$$
$$E_{1,1,3} = E_{1,3,1} = E_{3,1,1} = 11 \text{ (3-fold degenerate)}$$
$$E_{2,2,2} = 12 \text{ (nondegenerate)}$$
$$E_{1,2,3} = E_{1,3,2} = E_{2,1,3} = E_{2,3,1} = E_{3,1,2} = E_{3,2,1} = 14 \text{ (6-fold degenerate)}$$

Now, LHS of above equation is just a constant so we can write it as a $\frac{Z''(z)}{Z(z)} = -\gamma^2$ (6)

Thereby we have transformed a single Schrodinger equation (1) into three ordinary differential equations

$X''+\alpha^2 X = 0; Y''+\beta^2 Y = 0$ and $Z''+\gamma^2 Z = 0$

The constants α, β and γ are related by

$$\frac{2mE}{\hbar^2} = \alpha^2 + \beta^2 + \gamma^2 \qquad (7)$$

Each of the equations (4, 5 and 6) with its associated boundary conditions in (2) is equivalent to the one-dimensional problem. The normalized solutions X(x), Y (y), Z(z) can therefore be written down in complete analogy with one dimensional box

$$X_{n1}(x) = \left(\frac{2}{a}\right)^{1/2} Sin\frac{n_1\pi x}{a}; \quad n_1 = 1,2,3..... \qquad (8)$$

$$Y_{n2}(x) = \left(\frac{2}{a}\right)^{1/2} Sin\frac{n_2\pi y}{b}; \quad n_2 = 1,2,3.... \qquad (9).$$

$$Z_{n3}(x) = \left(\frac{2}{a}\right)^{1/2} Sin\frac{n_2\pi z}{c}; \quad n_3 = 1,2,3..... \qquad (10)$$

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