Lecture notes on Quantum Physics

Based on PH502 course in IIT Bhilai

MSc and BTech students, Instructor

Contents

Chapter 1

Scientific History of Light

Many researchers through the ages have taken up the challenge of finding out "What is Light?".Optics is known as the oldest discipline along with mechanics.The progress of the study of light has been made by the great scholars from different fields introduced here while leading other discipline and closely involved with the growth of industry and culture.

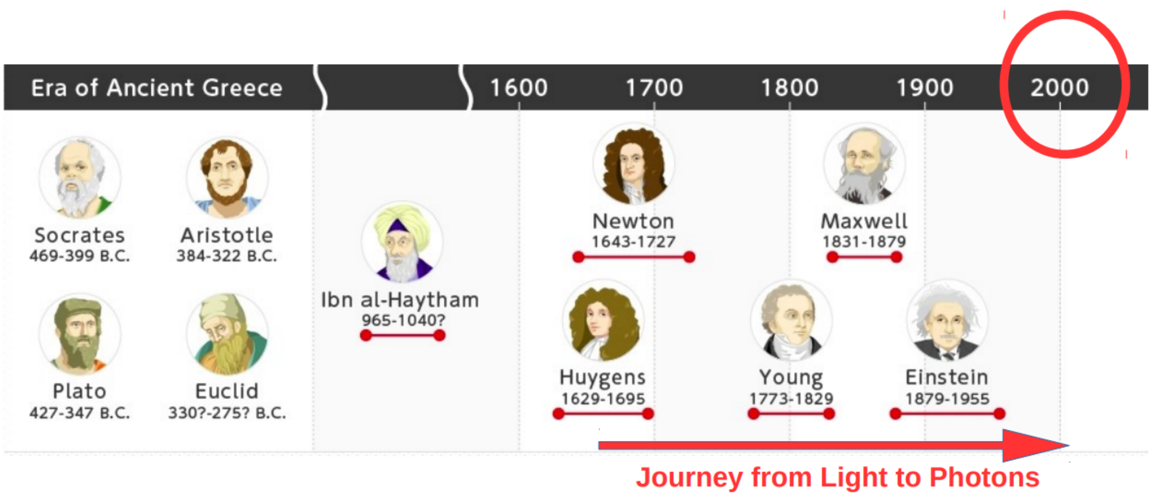


Figure 1.1: Journey from light to photons

[1] **Era of Ancient Greece-Aristotle(5th-3rd B.C.):**
The foundation for modern optics field was laid in ancient Greece in research carried out approximately 5^{th} B.C. to 3^{rd} B.C. The three great philosophers of ancient Greece or namely Socrates (469-399 B.C.), Plato (427-347 B.C.), and Aristotle (384-322 B.C.) established the foundations of the disciplines of astronomy, biology, mathematics, politics, and philosophy, etc.Then Euclid (330-275 B.C.) summarized fundamental knowledge of optics, such as reflection, diffusion and vision, into a book called "Optics".These concepts on light established in the age of Ancient Greece rendered a large effect up until the appearance of Newton in the late 17^{th} century.

"The essence of light is white light.Colors are made up of a mixture of lightness and darkness."

[2] **Ibn al-Haytham-Alhazen(965-1040):**

Born in the city of Basra in Iraq, Ibn al-Haytham was an active scholar in Basra and Cairo (Egypt).He made an intensive study of Grecian academics and left numerous writings to later generations. In the field of optics also,he left major historic works including the "Book of Optics" that covers experiments and observation on light reflection and refraction through the use of lenses and mirrors.He also authored treatises on reflection from concave mirrors, refraction from glass spheres, visual perception,light from the moon and stars,and the structure of space.His usage of precise theory through the application of mathematical methods and the experimental method served as the driving force for modern science.

"Why does the moon appear larger near the horizon than it does when higher up in the sky ?"

[3] **Sir Isaac Newton(1643-1727):**

Newton is credited with three major discoveries one of which was carrying out "Optical research into the spectral decomposition of light." (The others are "universal gravitation" and "infinitesimal calculus.") He greatly contributed to the development of the science of optics by collecting technology on lenses, prisms, mirrors, telescopes, microscopes and optical (mirror/lens) polishing. In 1668, he fabricated a reflecting telescope having no chromatic aberrations. In a paper presented in 1672, he announced his "New Theory on Light and Color" in which he proclaimed that "light is a mixture of various colors having different refractivity" rather than "the pure white (sunlight)" proposed by Aristotle, and demonstrated his theory in the famous prism experiment. In 1704, he authored the book "Opticks" where he reveals his "Light Particle Theory."

"Light is comprised of colored particles."

[4] **Christian Huygens(1629-1695):**

Christian Huygens was born in Hague in Netherlands.His father was a diplomat and politician.As an astronomer, he discovered Saturn's satellite Titan, the Saturn's ring, and the Great Nebula of Orion with a self-fabricated telescope of magnification of 50x. In 1690, he published a paper on light advocating his theory that light is a wave or wave-front. He utilized this theory of light as a wave to explain light reflection and refraction phenomenon. After repeated stormy debates opposing Newton's light particle theory, Huygens' theory that light is a wave became the mainstream scientific concept.

"Light is a wave."

[5] **Thomas Young(1773-1829):**

The accomplishments of Young extend to many fields including deciphering text from ancient Egypt, the theory on blood circulation, proposing the second pendulum, introducing Young's modulus into elasticity, and a multitude of others. In a shift of research from vision (trichromatic color vision and eye adjustment mechanism) to optics, in 1807 he showed that when light coming from a point light source is shined onto two pinholes, interference fringes can be observed on a screen an appropriate distance away

(Young's Experiment) and advocated his theory that light behaves like a wave. In the field of elastic body mechanics, his name still remains as the fundamental constant Young's Modulus, amongst other achievements he was first to use the term energy and introduced that concept.

"Proof of the wave theory of light"

[6] **James Clerk Maxwell(1831-1879):**

This scholar established the field of classical electrodynamics based on the famous Maxwell's Equations in 1864 that became the foundation for modern electromagnetism. The following four equations known as Maxwell's Equations have been called the "Jewel of Physics."He also theoretically predicted the existence of electromagnetic waves, the fact that electromagnetic waves propagate at the same speed as light, and as horizontal waves. He is further well known for his research on the composition of Saturn's rings and the Kinetic theory of gases (Maxwell-Boltzmann distribution).

"Predicted the existence of electromagnetic waves"

[7] **Albert Einstein(1879-1955):**

Einstein is called the greatest physicist of the 20^{th} century because of three groundbreaking research results announced in 1905 that had a great impact on physics. Those three papers were on the photoelectric effect theory where light is made up of particles called photons, the theory of Brownian motion utilizing kinetic theory of molecules, and the theory of special relativity. The theory of relativity in particular was a new discovery about space and time expressed in the relativity principle of electromagnetism and which resolved the ether problem in 19^{th} century physics. Einstein is famous for his research on the theory of relativity yet his work on theoretically revealing the photoelectric effect based on the light quantum hypothesis won him the Nobel Prize in physics in 1921.

"Light is a photon"

Through the researches accumulated over 2,000 years of time, the true nature of light or namely the photon was discovered. The photon has many mysterious physical properties such as possessing the dual properties of a wave and a particle. Revealing facts of these properties may lead us to using light more effectively than ever before.

Chapter 2

Photo electric effect

Work Function(W): It is defined as the minimum energy required to liberate an electron from the metal surface.

W = ($h\nu_o$) where ν_o = Threshold Frequency.
N_{Photon}(h$\nu - h\nu_o$)= $N_{electron}(1/2)mv^2$ = eV.

where,
N = Number of Photons.
h = Planck's Constant.
m = Mass of electron.
v = velocity of electron liberated.
V = Stopping Potential.

Since,
$eV_o = \frac{mv_{max}^2}{2}$.
$h\nu - h\nu_o = eV_o$.
V_o = $(\frac{h}{e})\nu$ - $(\frac{h}{e})\nu_o$ where, $\frac{h}{e}\nu_o$ = Constant.
In fig.(a), $I_1 > I_2 > I_3$ where, I is the intensity of Light.

Experimental Facts :

1] Classical View. 2] Quantum View(Light = hν).

[1]

Work done = Power * Time

Work done = # $|E|$ * Time = Work Function. $\rightarrow$ From quantum view it is an instantaneous process.

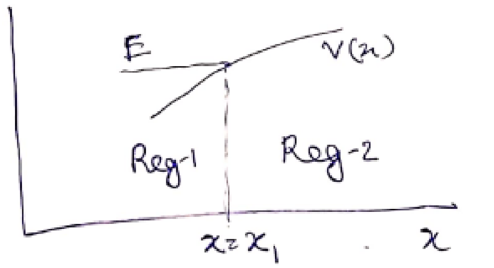
But from experiment, it is observed that it takes few weeks to create photo current.

[2]

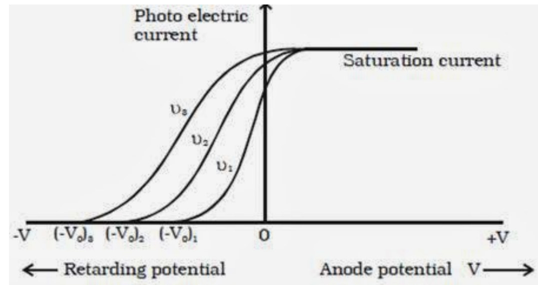
Intensity of Light = # $|E| \uparrow$.
$\implies$ Work Done $\uparrow$.
$\implies$ (Work Done - W) = $\frac{mv^2}{2}$ = Kinetic Energy $\uparrow$.

But Kinetic Energy is independent of intensity of light from quantum point of view.

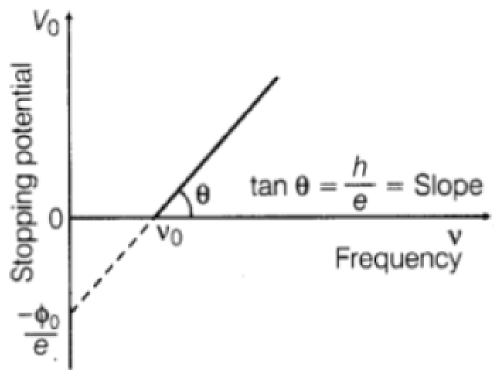
[3]



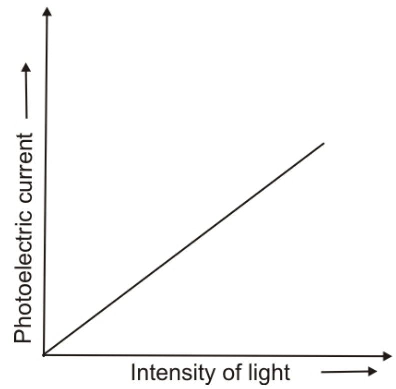
(a) Photoelectric current vs Anode Potential



(b) Photoelectric Current vs Anode Potential



(c) Stopping potential vs Frequency



(d) Photo Current vs Intensity of Light

Classical View failed to explain why ν_o comes into picture but when we consider the equation $[Energy = h * frequency]$ then we can understand from Einstein's relation.

Chapter 3

Black body radiation

What is a blackbody ?

A body which absorbs incident radiation of all wavelength but does not transmit it or reflect it is called a blackbody. A black body is an idealized physical body that absorbs all incident electromagnetic radiation, regardless of frequency or angle of incidence. The name black body is given because it absorbs all colors of light. The black body also emits black body radiation.

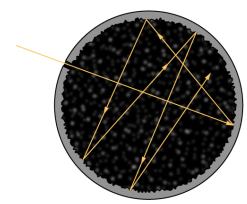


Figure 3.1: black body absorbs all the light

What is blackbody radiation?

When a matter heated its emits radiation of different wavelengths and when a black body is heated up and kept at a fixed temperature than em radiation are emitted from inner wall of blackbody. After some the cavity is filled up by the radiation. In a dark room, a black body at room temperature appears black because most of the energy it radiates is in the infrared spectrum and cannot be perceived by the human eye.

The black body radiation is characterised as

1. Isotropic and non-polarized
2. Independent of shape of cavity
3. Depends only on temperature
4. In perfect black body emisivity is equal to unity due to thermodynamic equilibrium
5. The spectral energy density for each wavelength increases with temprature

After observing the blackbody radiation curve people started to work to find expressions to fit the curve. They all started with the classical idea to explain the curve but failed . Lets look at the ideas one by one

3.1 Weins Distribution Law

Wien's distribution is a law of physics used to describe the spectrum of thermal radiation (frequently called the blackbody function). This law was first derived by Wilhelm Wien in 1896. The equation does accurately describe the short wavelength (high frequency) spectrum of thermal emission from objects, but it fails to accurately fit the experimental

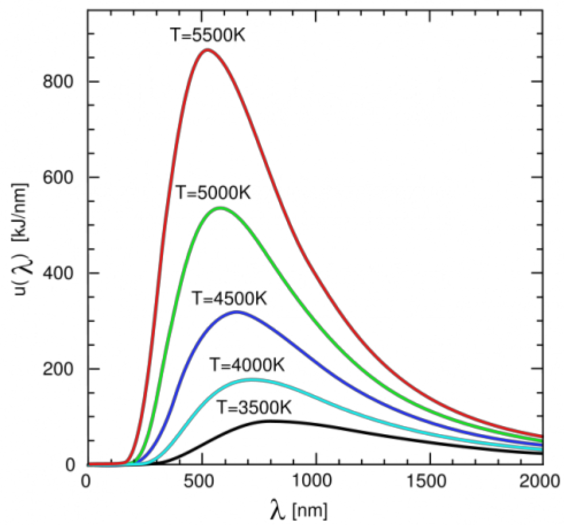


Figure 3.2: experimental curve of black boby radiation for different temperatures

data for long wavelengths (low frequency) emission.

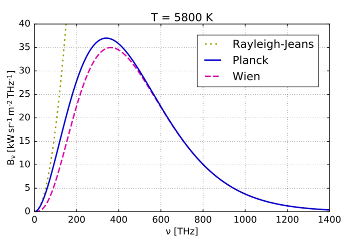


Figure 3.3: comparison of of Rayleigh-jeans,Plancks and weins law

The pink dotted line is for wiens law which does not fit the curve at low frequency as seen but completely satisfies the curve at high frequencies.
To fit the curve weins deduced the following equation

$$E_\lambda d\lambda = \frac{a}{\lambda^5} \exp(-b/\lambda T) d\lambda \tag{3.1}$$

This equation satisfies the curve at low wavelength(high frequencies).

Here E_λ is the emmisive power which is defined as the energy emitted per unit area per unit time per unit λ

From above equation one can deduce weins displacement law by differentiating it which is

$$\lambda_{max} T = constant \tag{3.2}$$

Wien's displacement law states that the black-body radiation curve for different temperatures will peak at different wavelengths that are inversely proportional to the temperature. The value of weins constant is= 2.897771955×10^-3 m K

(Example) Wein's law gives us relationship between wavelength of light that correspond to the highest intensity and the absolute temperature of object that emits the radiation. suppose that a distant star has a surface temperature of $25000k$. What color is that the light it emits?
(Answer) from wein's law we know

$$\lambda_{max} T = constant \tag{3.3}$$

The value of weins constant is= 2.897771955×10^-3 m K

$$\lambda_{max}T = 2.897771955 \times 10^-3 \tag{3.4}$$

$$\lambda_{max} = 2.897771955 \times 10^-3/T \tag{3.5}$$

$$\lambda_{max} = \frac{2.897771955 \times 10^-3}{25000} \tag{3.6}$$

$$\lambda_{max} = 116nm \tag{3.7}$$

So it is fall into the ultraviolet radiation
and in the visible region blue light will have the greatest intensity ans so it is the color we observe for the star.

3.2 Rayleigh-jeans law

Another person who tried to explain the black body curve was Reyleigh-jeans. He assumed the following assumptions
1. He assumed the standing waves in the cavity.
2. He stated that the standing waves are in harmonic motion and follows the law of Equipartition of Energy i.e. half of (KT) energy is equal to Kinetic Energy and half of (KT) energy is equal to Potential Energy.
3. No. of oscillators of(standing waves)per unit volume in range of ν to $\nu + d\nu$ is $2 * \frac{4\pi\nu^2 d\nu}{c^2} = n_\nu d\nu$
4. Energy of each oscillator is $\epsilon = K_b$T; where K_b is boltzmann constant and T is temperature.So

$$\begin{aligned} E_\nu d\nu &= \epsilon n_\nu d\nu \\ &= KT\frac{8\pi\nu^2 d\nu}{c^3} \end{aligned} \tag{3.8}$$

In terms of wavelength it can be written as

$$E_\lambda d\lambda = \frac{8\pi KT d\lambda}{\lambda^4} \tag{3.9}$$

As we go towards the shorter wavelength i.e in ultraviolet end of spectrum, energy density also increases by above formula and the energy increases at very rate and it tends towards infinity.But in reality energy density should approach 0 as $\nu \to \infty$. This discrepancy is known as the Ultraviolet Catastrophe of classical physics.So the major drawback of Rayleigh-jeans law was that it was applicable only for higher wavelength.
Where did Rayleigh -Jeans go wrong?

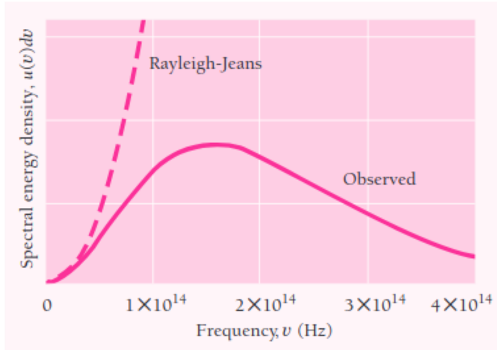


Figure 3.4: comparison of reyleigh-jeans vs observed curve

3.3 Plank's Radiation Formula

Additional assumptions:- Energies are quantified/Discrete.

$e.g.\mathcal{E}, 2\mathcal{E}, 3\mathcal{E}, 4\mathcal{E}....r\mathcal{E}....$

Total no. of Plank oscillator

$$N = N_0 + N_1 + N_2 + ... + N_r + ... \tag{3.10}$$

here $N_r = N_0 e^{-\mathcal{E}_r/KT}$

$$N = N_0 + N_0 e^{-\mathcal{E}/KT} + N_0 e^{-2\mathcal{E}/KT} + ... + N_0 e^{-r\mathcal{E}/KT} + ... \tag{3.11}$$

$$= N_0[1/(1 - e^{-\mathcal{E}/KT}]//asx = e^{-\mathcal{E}/KT} << 1 \tag{3.12}$$

$$E = E_0 + E_1 + E_2 + ... + E_r + ... \qquad \text{(Total energy)} \tag{3.13}$$

$$E = 0 + \mathcal{E}N_1 + 2\mathcal{E}N_2 + ... + r\mathcal{E}N_r + ...$$

$$= N_0[\epsilon e^{-\mathcal{E}/KT} + 2\mathcal{E}e^{-2\mathcal{E}/KT} + ... + r\mathcal{E}e^{-r\mathcal{E}/KT} + ...]$$

$$= N_0 e^{-\mathcal{E}/KT}[1 + 2x + 3x^2 + ... + rx^{r-1} + ...]$$

$$= N_0 e^{-\mathcal{E}/KT}/(1 - N_0 e^{-\mathcal{E}/KT})^2 \tag{3.14}$$

$$\frac{d}{dx}\left(\frac{1}{1-x}\right) = \frac{d(1 + x + x^2 + x^+ .... + x^r + ...)}{dx}$$

$$\frac{1}{-x^2} = (1 + 2x + 3x^2 + ... + rx^{r-1} + ...)$$

So average energy

$$\mathcal{E} = E/N = \mathcal{E}e^{-\epsilon/KT}/(1 - e^{-\epsilon/KT}) = \mathcal{E}/(e^{\mathcal{E}/KT} - 1) \tag{3.15}$$

Plank's also assumed the following relation:

$$E = h\nu \qquad \bar{\epsilon} = \frac{h\nu}{(e^{h\nu/KT} - 1)}$$

$$E_\nu d\nu = [\frac{8\pi\nu^3 d\nu}{c^3}][\frac{h\nu}{e^[(h\nu)/kT] - 1}]$$

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}(\frac{1}{e^{hc/\lambda KT} - 1})d\lambda \tag{3.16}$$

3.4 Plank's law in limiting case

$$E_\lambda = 8\pi hc/\lambda^5(\frac{1}{e^{hc/\lambda KT} - 1}) \tag{3.17}$$

when λ is small $\frac{he}{\lambda KT}$ will be large so $(\frac{1}{e^{hc/\lambda KT}-1}) = e^{-hc/\lambda KT}$
So,

$$E_\lambda = \frac{8\pi hc}{\lambda^5}e^{-hc/\lambda KT} = \frac{Ae^{-B/\lambda T}}{\lambda^5} \quad (\text{ Wien's law }) \tag{3.18}$$

when λ is large $\frac{he}{\lambda KT}$ will be small

$$\frac{1}{e^{hc/\lambda KT} - 1} = \frac{1}{1 + hc/\lambda KT - 1} = \frac{\lambda KT}{hc}$$

So,

$$E_\lambda = \frac{8\pi hc}{\lambda^5}\frac{\lambda KT}{hc} = \frac{8\pi KT}{\lambda^4}(\text{Rayleigh-jeans law}) \tag{3.19}$$

Chapter 4

QM explanation of Black body radiation

Electromagnetic wave is reflected from the surface of a good conductor. Hence it is possible to store electromagnetic waves in a cavity, in terms of standing waves. As there is no net energy transport out of the cavity the waves inside can be treated as a standing wave. Standing waves are a result of reflection and interference and appear to exhibit simple harmonic motion.

4.1 Equation of EM-Wave trapped in a cavity

Considering a cubical cavity of side L with perfectly conducting walls, containing a perfect vacuum. Wave equation for the electric field inside he cavity is given by-

$$\nabla^2 \vec{E} - \frac{1}{c^2} \cdot \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \tag{4.1}$$

Boundary Conditions

$$E_{\parallel} = 0 \tag{4.2}$$

$E_{\parallel}$ is the component of electric field parallel to the walls of the component.thus our solution should be such that it should satisfy the differential equation as well as the boundary condition. The general form of the solution will be -

$$\vec{E}(x, y, z, t) = \vec{E}_{\vec{r}} \cdot \exp -i.w.t \tag{4.3}$$

where $\vec{E}_{\vec{r}} = \vec{E}_{\vec{r}}(x, y, z)$ is a vector function of position(i.e. independent of time). Substituting the eqn.4.3 into eqn.4.1 we get -

$$\nabla^2 \vec{E}_{\vec{r}} + \frac{\omega^2}{c^2} \cdot \vec{E}_{\vec{r}} = 0 \tag{4.4}$$

Using separation of variable we can obtain the solution.The solution will be of the form as given below. The constants in the equation given below can be obtained by applying the boundary conditions, as well as substituting it back into the main equation.

$$E_x = E_{x_0} \cdot \cos(k_x.x)\sin(k_y.y) \cdot \sin(k_z.z) \cdot e^{-i.w.t} \tag{4.5}$$

$$E_y = E_{y_0} \cdot \sin(k_x.x)\cos(k_y.y) \cdot \sin(k_z.z) \cdot e^{-i.w.t} \tag{4.6}$$

$$E_z = E_{z_0} \cdot \sin(k_x.x)\sin(k_y.y) \cdot \cos(k_z.z) \cdot e^{-i.w.t} \tag{4.7}$$

In a similar way solving the differential equations of magnetic field and applying the boundary condition -

$$B_\perp = 0 \tag{4.8}$$

Consider two waves of same amplitude and wavelength that are travelling in opposite direction on a string.The resulting displacement of the string is given by

$$\begin{aligned} y(x,t) &= A \cdot \sin(k.x - \omega.t) + A \cdot \sin(k.x + \omega.t) \\ y(x,t) &= 2 \cdot A \cdot \sin(k.x) \cdot \cos(\omega.t) \end{aligned} \tag{4.9}$$

As the position and time the time dependence terms have separated it no longer represents a travelling wave. It can now be treated as a standing wave. Comparing eqn.4.5,eqn.4.6,eqn.4.7 with eqn.4.9 we can observe a similar separation of time and position dependence terms, resulting in the electromagnetic wave inside the cavity to be treated as a standing wave.
For eqn.4.5,eqn.4.6,eqn.4.7 to satisfy the wave equation the corresponding components of wave vectors must satisfy the following relations-

$$k_x^2 + k_y^2 + k_z^2 = \frac{\omega^2}{c^2} \tag{4.10}$$

But Wave vector $\vec{k}$ can also be written in Cartesian form in the following way-

$$\begin{aligned} \vec{k} &= k_x\hat{i} + k_y\hat{j} + k_z\hat{k} \\ |\vec{k}| &= k_x^2 + k_y^2 + k_z^2 \\ k^2 &= k_x^2 + k_y^2 + k_z^2 \end{aligned} \tag{4.11}$$

Substituting eqn.4.11 in eqn.4.10 we obtain the following relation between angular frequency ω and wave vector $\vec{k}$ which is given by-

$$\begin{aligned} k &= \frac{\omega}{c} \\ \omega &= k \cdot c \end{aligned} \tag{4.12}$$

Maxwell's equation given by-

$$\nabla \cdot \vec{E} = 0 \tag{4.13}$$

imposes the following constraint on the eqn.4.5,eqn.4.6,eqn.4.7 which gives us following relation between k and E.

$$k_x \cdot E_{x_0} + k_y \cdot E_{y_0} + k_z \cdot E_{z_0} = 0 \tag{4.14}$$

Applying boundary conditions to electric field component in y direction along x-axis-

$$E_y = 0 \text{ for } \begin{cases} x = 0 \\ x = L \end{cases} \quad \text{for all values of y, z, and t} \tag{4.15}$$

we get the following equation $k_x{\cdot}L = n_x{\cdot}\pi$.Similarly applying boundary conditions to x and z component of electric field we get-

$$k_x = \frac{n_x{\cdot}\pi}{L} \tag{4.16}$$

$$k_y = \frac{n_y{\cdot}\pi}{L} \tag{4.17}$$

$$k_z = \frac{n_z{\cdot}\pi}{L} \tag{4.18}$$

where n_x, n_y, n_z are integers and are referred to as a mode of oscillation for the electromagnetic wave within the cavity. Thus we can represent each mode of vibration by this triplet of integers.

4.2 Density state of an Electromagnetic Wave

An allowed mode of oscillation can be represented by a point in a three dimensional k-space. Each of these points is uniformly distributed with a spacing of $\frac{\pi}{L}$ between any two consecutive points. Volume occupied by a lone point in 3-D k-space is given by V_{ps}-

$$V_{ps} = \frac{\pi}{L}{\cdot}\frac{\pi}{L}{\cdot}\frac{\pi}{L}$$

$$V_{ps} = \left(\frac{\pi}{L}\right)^3 \tag{4.19}$$

Magnitude of the wave vector is given by $|k|$. Permitted modes of vibration with wave vector whose magnitude lies between k and $k + dk$,lie on one octant of spherical shell of radius k and thickness dk.We are considering only the positive values of k because of the choice of selection of coordinates. Volume of the shell is given by V_s

$$V_s = \frac{1}{8}{\times}4\pi k^2 dk \tag{4.20}$$

Allowed states with a wave vector whose magnitude lies between k and $k + dk$ is given by a function called $g(k)dk$ where $g(k)$ is known as density of states.

$$g(k)dk = \frac{\text{Volume in k-space of one octant of a spherical shell}}{\text{Volume in k-space occupied per allowed state}}$$

$$g(k){\cdot}dk = \frac{4\pi k^2}{\left(\frac{2\pi}{L}\right)^3}dk \tag{4.21}$$

However as an electromagnetic wave can be polarized in both the directions, so the eqn.4.21 needs to be multiplied by 2.

$$\begin{aligned}
g(k)\cdot dk &= \frac{4\pi k^2 \times 2}{\left(\frac{2\pi}{L}\right)^3} dk \\
g(k)\cdot dk &= \frac{V\cdot k^2}{(\pi)^2} dk \qquad \text{for } V = L^3 && (4.22) \\
k &= \frac{\omega}{c} \qquad => \qquad \frac{dk}{d\omega} = \frac{1}{c} \\
g(\omega) &= g(k)\frac{dk}{d\omega} \qquad => \qquad g(\omega) = \frac{1}{c} g(k) \\
g(\omega) d\omega &= \frac{V\cdot\omega^2}{\pi^2\cdot c^3} d\omega && (4.23)
\end{aligned}$$

4.3 Electromagnetic wave as an simple Harmonic Oscillator

The electromagnetic wave trapped in a cavity can be treated as an Simple harmonic oscillator as was previously explained in Section-4.1. Lets now derive and reconcile the relations that we know for simple harmonic oscillator with the expressions that we have derived for a trapped EM-wave. For a simple harmonic oscillator the energy of the system is given by-

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{4.24}$$

The partition function of a system with energy E_α is given by-

$$Z = \sum_\alpha e^{-\beta E_\alpha} \qquad \text{where } \beta = \frac{1}{k_\beta T} \tag{4.25}$$

So a partition function of the simple harmonic oscillator system is given by-

$$\begin{aligned}
Z &= \sum_{n=0}^{\infty} e^{-\beta\left(n+\frac{1}{2}\right)\hbar\omega} \\
&= e^{-\beta\frac{\hbar\omega}{2}} \cdot \sum_{n=0}^{\infty} e^{-\beta n\hbar\omega} \\
Z &= e^{-\beta\frac{\hbar\omega}{2}} \cdot \left[1 + \frac{1}{e^{\beta\hbar\omega}} + \frac{1}{e^{2\beta\hbar\omega}} + \frac{1}{e^{3\beta\hbar\omega}} + ...\right] && (4.26)
\end{aligned}$$

The term given in square brackets represents a geometric progression with the first term being 1 and the common ratio being given by $e^{-\beta\hbar\omega}$. Thus partition function of the system can be written as

$$Z = \left[\frac{e^{-\beta\frac{\hbar\omega}{2}}\cdot}{1 - e^{-\beta\hbar\omega}}\right] \tag{4.27}$$

Internal energy (U) of the system can be obtained from the partition function in the following way-

$$\begin{aligned} U &= -\frac{d \ln z}{d\beta} \\ &= \hbar\omega \left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1} \right) \end{aligned} \tag{4.28}$$

4.4 Reconciling SHM with EM-wave trapped in a cavity

The above expression is for the case of harmonic oscillator with single angular frequency. However in our case due to presence of the multiple angular frequencies owing to the different modes of oscillation of the system, we need to take into consideration the density of state of the system to obtain the spectral distribution of the internal energy of the system.

$$\begin{aligned} U &= \int_0^\infty g(\omega) d\omega \times \hbar\omega \left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1} \right) \\ &= \left(\int_0^\infty \frac{1}{2} \hbar\omega \times g(\omega) d\omega \right) + \left(\int_0^\infty \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \times g(\omega) d\omega \right) \end{aligned} \tag{4.29}$$

The first part of the equation diverges due to presence of the zero-point energy terms.This issue can be resolved by redefining or reference for zero point energy, such that the first term is absorbed is absorbed/eliminated.Thus we obtain-

$$\begin{aligned} U &= \int_0^\infty \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \times g(\omega) d\omega \\ &= \frac{V\hbar}{\pi^2 c^3} \int_0^\infty \frac{\omega^3 d\omega}{e^{\beta\hbar\omega} - 1} \end{aligned} \tag{4.30}$$

The spectral energy density (u) of the black body in term of energy density (U) is given by -

$$u = \frac{U}{V} = \int u_\omega d\omega \tag{4.31}$$

Equating eqn.**??** and eqn.4.31 we get

$$u_\omega = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{e^{\beta\hbar\omega} - 1} \tag{4.32}$$

$$\omega = 2\pi\nu \qquad => \qquad d\omega = 2\pi d\nu$$

$$u_\omega d\omega = u_\nu d\nu$$

$$\boxed{u_\nu = \frac{8\pi h}{c^3} \frac{\nu^3}{e^{\frac{h\nu}{k_B T}} - 1}} \quad \text{Black-Body distribution function in terms of frequency}(\nu) \tag{4.33}$$

We can obtain the black body distribution function with wavelength being the subject of the equation in a similar way

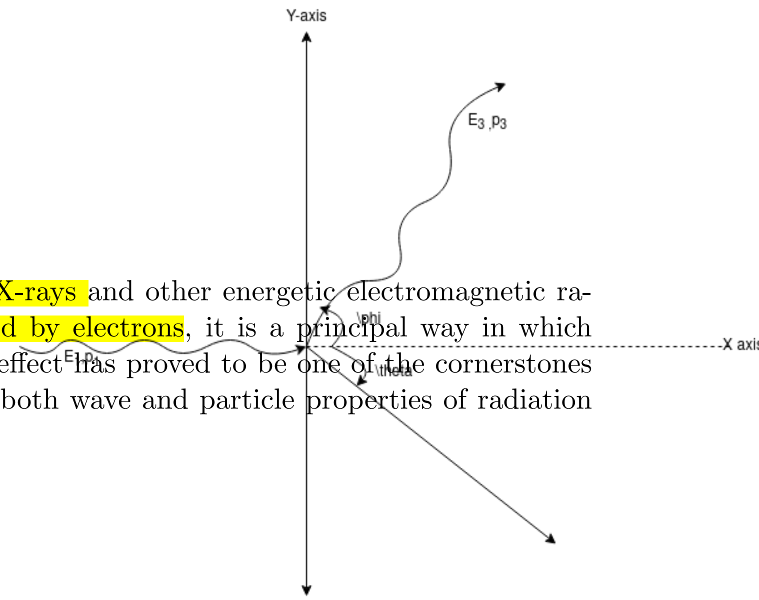
$$\nu = \frac{c}{\lambda} \qquad => \qquad \frac{d\nu}{d\lambda} = \frac{-1}{\lambda^2}$$

$$u_\nu |d\nu| = u_\lambda |d\lambda|$$

$$\boxed{u_\lambda = \frac{8\pi hc}{\lambda^5}\frac{\nu^3}{e^{\frac{hc}{\lambda k_B T}}-1}} \quad \text{Black-Body distribution function in terms of wavelength}(\lambda) \tag{4.34}$$

Chapter 5

Compton Effect



Compton effect, increase in wavelength of X-rays and other energetic electromagnetic radiations that have been elastically scattered by electrons, it is a principal way in which radiant energy is absorbed in matter. The effect has proved to be one of the cornerstones of quantum mechanics, which accounts for both wave and particle properties of radiation as well as of matter.

$E_1 = h\nu$ $p_1 = \frac{h\nu}{c}$ $E_3 = h\nu'$ $p_3 = \frac{h\nu'}{c}$

$$(E_1, P_1)$$
$$(E_2 = m_0c^2, p_2 = 0)$$
$$\downarrow Collision$$
$$(E_3, P_3)$$
$$(E_4 = mc^2 = \sqrt{p^2c^2 + m_0^2c^4}, P_4 = p)$$

Momentum conservation:-

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c}cos(\phi) + pcos(\theta) \text{ (along x-axis)---eqn(1)}$$
$$0 = \frac{h\nu'}{c}sin(\phi) - psin(\theta) \text{ (along y-axis)---eqn(2)}$$
$$\implies p^2c^2(sin^2\theta + cos^2\theta) = (h\nu - h\nu' cos\phi)^2 + (h\nu' sin\phi)^2$$
$$\implies p^2c^2 = (h\nu)^2 + (h\nu')^2 - 2(h\nu)(h\nu')cos\phi$$

Energy conservation:-

$$h\nu + m_0c^2 = h\nu' + \sqrt{p^2c^2 + m_0^2c^4} \text{ ---eqn(3)}$$
$$\implies p^2c^2 + m_0^2c^4 = ((h\nu - h\nu') + m_0c^2)^2$$
$$\implies p^2c^2 + m_0^2c^4 = (h\nu - h\nu')^2 + 2(h\nu - h\nu')m_0c^2 + m_0^2c^4$$
$$\text{using result of } eq^n \text{ 1 and 2}$$
$$\implies ((h\nu)^2 + (h\nu')^2 - 2(h\nu)(h\nu')) + 2(h\nu - h\nu')m_0c^2 = p^2c^2 =$$
$$(h\nu)^2 + (h\nu')^2 - 2(h\nu)(h\nu')cos(\phi)$$

$$\implies 2(h\nu)(h\nu')(1-cos(\phi)) = 2(h\nu - h\nu')m_0c^2$$
$$\implies \tfrac{h}{m_0c}(1-cos(\phi)) = \tfrac{c(\nu-\nu')}{\nu\nu'}$$
$$\implies (\lambda'-\lambda) = \tfrac{h}{m_0c}(1-cos(\phi)) \text{ and } \Delta\lambda = (\lambda'-\lambda) = \text{Compton shift}$$
$$\tfrac{h}{m_0c} = \lambda_0 = \text{Compton wave length}$$

Energy of recoil electron:
We see $\nu' = \frac{\nu}{1+2\alpha\sin^2\frac{\phi}{2}} \quad \alpha = \frac{h\nu}{m_0c^2}$
Electron enengy (kinetic) $= mc^2 - m_0c^2 = h\nu - h\nu'$

$$E = h\nu - \frac{h\nu}{1+2\alpha\sin^2\frac{\phi}{2}}$$

$$= \frac{h\nu 2\alpha\sin^2\frac{\phi}{2}}{1+2\alpha\sin^2\frac{\phi}{2}} = hv\left[\frac{2\alpha\sin^2\frac{\theta}{2}}{1+2\alpha\sin^2\frac{\Phi}{2}}\right]$$

$$E_{\min} = 0,\ \Delta\lambda = \frac{h}{m_0C}(1-\cos\phi) = 0,\ \text{ and } \nu' = \nu, \lambda' = \lambda$$

$$\sin^2\frac{\pi}{4} = \frac{1}{2} \Rightarrow E = \left(\frac{\alpha}{1+\alpha}\right)h\nu$$

$$\lambda' - \lambda = \frac{h}{m_0c} \Rightarrow \lambda' = \lambda + \frac{h}{m_0c} \text{ and } v' = \frac{\nu}{1+\alpha}$$

$$\sin^2\frac{\pi}{2} = 1 \Rightarrow E_{\max} = \left(\frac{2\alpha}{1+2\alpha}\right)h\nu$$

$$\lambda' = \frac{2h}{m_0c} \quad and \quad \nu' = \frac{\nu}{1+2\alpha}$$

$$\frac{2\alpha}{1+2\alpha} < 1 \Rightarrow E_{\max} < h\nu$$

Direction of Recoil Electron:
From above two equations, we get

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c}cos\phi + pcos\theta \tag{5.1}$$

$$0 = \frac{h\nu'}{c}sin\phi - psin\theta \tag{5.2}$$

$$\implies tan\theta = \frac{\frac{h\nu'}{c}sin\theta}{\frac{h\nu}{c} - \frac{h\nu'}{c}cos\phi} \tag{5.3}$$

Now from compton shift relation,

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_oc}(1-cos\phi)$$

$$\implies \frac{c}{\nu'} - \frac{c}{\nu} = \frac{h}{m_oc}(1-cos\phi)$$

$$\implies \frac{1}{\nu'} = \frac{c}{\nu} + \frac{h}{m_o c^2}(1 - cos\phi)$$

$$\implies \nu' = \frac{1}{\frac{1}{\nu} + \frac{h}{m_o c^2} 2sin^2\frac{\phi}{2}}$$

$$\implies \nu' = \frac{\nu}{1 + \frac{h\nu}{m_o c^2} 2sin^2\frac{\phi}{2}} \tag{5.4}$$

Using 5.4 in 5.3, we get

$$tan\theta = \frac{(\frac{\nu}{1+2\alpha sin^2\frac{\phi}{2}})sin\phi}{\nu - (\frac{\nu}{1+2\alpha sin^2\frac{\phi}{2}})cos\phi}$$

$$\implies \frac{sin\phi}{1 + 2\alpha sin^2\frac{\phi}{2} - cos\phi} = \frac{2sin\frac{\phi}{2}cos\frac{\phi}{2}}{2\alpha sin^2\frac{\phi}{2} + 2sin^2\frac{\phi}{2}}$$

Hence,

$$tan\theta = \frac{cot\frac{\phi}{2}}{1+\alpha} \tag{5.5}$$

where $\alpha = \frac{h\nu}{m_0 c^2}$

Chapter 6

Matter wave

Matter waves are a central part of the theory of quantum mechanics, being an example of wave–particle duality. All matter exhibits wave-like behavior. For example, a beam of electrons can be diffracted just like a beam of light or a water wave. In most cases, however, the wavelength is too small to have a practical impact on day-to-day activities.

The concept that matter behaves like a wave was proposed by French physicist Louis de Broglie in 1924. It is also referred to as the de Broglie hypothesis. Matter waves are referred to as de Broglie waves.

6.1 Wave Nature of Particle

According to De Broglie hypothesis,

$$\lambda = \frac{h}{p} \tag{6.1}$$

Now, for non-realistic particle with Kinetic Energy, $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$,

$$\lambda = \frac{h}{\sqrt{2mE}} \tag{6.2}$$

Substituting, $E = \frac{1}{2}mv^2$ with ev, we get:

$$\lambda = \frac{h}{\sqrt{2mev}} \implies \lambda = (\frac{h}{\sqrt{2me}})\frac{1}{\sqrt{v}}$$

Substituting, the values of h, m and e, we get:

$$\lambda = \frac{h}{\sqrt{2me}} = \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}}}$$

$$\lambda \approx 12.26 \times 10^{-10} m$$

Thus, we get:

$$\lambda = \frac{12.26}{\sqrt{v}} \mathring{A} \tag{6.3}$$

6.2 Relativity

We know that,

$$E = \frac{p^2}{2m} \tag{6.4}$$

And, we know that $E_{total} = E_k + m_o c^2$, where $m_o c^2$ is the rest mass energy. Also,

$$m(v) = \frac{m_o}{\sqrt{1 - \frac{v^2}{c^2}}} \approx m_o$$

when, $\frac{v}{c} << 1 \implies (1 - \frac{v^2}{c^2})^{\frac{1}{2}} = 1 - \frac{1}{2}(\frac{v^2}{c^2}) + \frac{(-\frac{1}{2})(\frac{1}{2}-1)(\frac{v^2}{c^2})}{2!}... \approx 1$

$$E_{total} = \sqrt{p^2c^2 + m_o^2 p^4}$$

$$\implies E_t^2 = p^2c^2 + m_o^2 p^4 = (E_k + m_o c^2)^2$$

$$\implies p^2c^2 = E_k(E_k + 2m_o c^2)$$

$$\implies p = \frac{\sqrt{E_k(E_k + 2m_o c^2)}}{c} \tag{6.5}$$

We know that, De Broglie Wavelength $\lambda = \frac{h}{p}$. Thus, for realistic particles, with Kinetic Energy, E_k, we get:

$$\lambda = \frac{hc}{\sqrt{E_k(E_k + 2m_o c^2}} \tag{6.6}$$

When, $E_k = eV = (E_t - m_o c^2)$, then

$$\lambda = \frac{hc}{\sqrt{ev(ev + 2m_o c^2}} \tag{6.7}$$

6.3 WBUT-2010

1] viii) If $E_t >> m_0 c^2$

$$E_t = \sqrt{p^2c^2 + m_0^2 e^4} \approx pc$$

$$or(pc >> m_0 c^2)$$

$$E_t \quad \alpha \quad p$$

5] a) v= 50% of c

$$v = \frac{c}{2}$$

$$v = 1.5x10^8$$

$$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$= \frac{m_0}{\sqrt{1-\frac{1}{4}}}$$

(where $m_0 = 9.1x10^{-31}kg$)

$$p = mv$$

$$p = \frac{m_0 c}{\sqrt{3}}$$

$$E_{tot} = \sqrt{p^2c^2 + m_0^2c^4}$$

$$= m_0c^2\frac{2}{\sqrt{3}}$$

$$or \quad E_{tot} = mc^2$$

$$= \frac{2}{\sqrt{3}}m_0c^2$$

So, K.E, $E_k = E_{tot} - m_0c^2$

$$= (\frac{2}{\sqrt{3}} - 1)m_0c^2$$

WBUT-2011

1(X): $m_{He} > m_p > m_e$, $\nu_{He} = \nu_p = \nu_e$.

$\rightarrow \lambda = h/mv \Rightarrow \lambda_e > \lambda_p > \lambda_{He}$ for NR or R.

1(Xii): $KineticEnergy \quad E_K = m_oc^2$

$$\rightarrow E_{tot} = E_k + m_oc^2 = mc^2$$

$$\Rightarrow m = 2m_o$$

10(c): $E = mc^2$ when $v << c$, $E_k = \frac{1}{2}m_ov^2$

$$E = \frac{m_oc^2}{(1-\frac{v^2}{c^2})^{\frac{1}{2}}}$$

$$E = m_oc^2(1-\frac{v^2}{c^2})^{\frac{-1}{2}}$$

$$E = m_oc^2[1 + \frac{v^2}{2c^2} - \frac{(-\frac{1}{2})(-\frac{1}{2}-1)}{2!}(\frac{v^2}{c^2})^2 + ...]$$

$$E \approx m_oc^2 + \frac{1}{2}m_ov^2$$

$$E = m_o c^2 + E_k$$

$$\Rightarrow E_k = \frac{1}{2} m_o v^2$$

$$E = [m_o^2 c^4 + p^2 c^2]^{\frac{1}{2}}$$

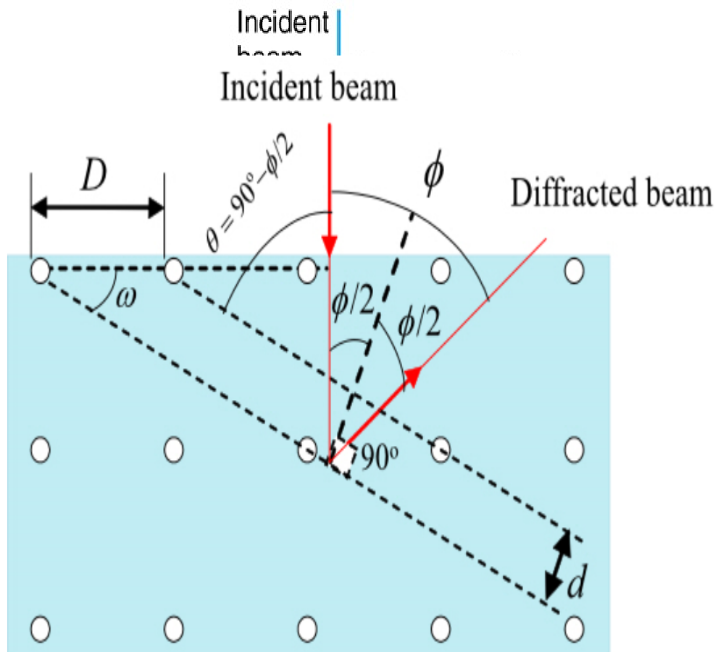
$$E = m_o c^2 [1 + \frac{p^2 c^2}{m_o^2 c^4}]^{\frac{1}{2}}$$

$$E = m_o c^2 [1 + \frac{1}{2}\frac{p^2 c^2}{m_o^2 c^4} + \frac{1}{2}($$

$$E = m_o c^2 + \frac{p^2}{2m_o}$$

Devision-Germer's experiment:
The Davisson–Germer experiment was a 19 Lester Germer at Western Electric (later Bel surface of a crystal of nickel metal, displaye hypothesis, advanced by Louis de Broglie ir experimental milestone in the creation of qua

$$2dsin$$



Since

$$d = Dsin\alpha$$

$$sin\theta = sin(90 - \alpha) = cos\alpha$$

Thus

$$2Dsin\alpha cos\alpha = \lambda$$

$$Dsin2\alpha = \lambda = h/\sqrt{2meV}$$

for d = 2.15 angstrom, $2\alpha = 50^\circ = \lambda = 1.65$ angstrom

Probability of particle in position x = $|\psi(x)|^2$

For electron: v = 10^6 m/s

m = $9 * 10^{-31}$ kg

$\lambda = 10$ angstrom

For bullet: v = 10^3 m/s

m = 10^{-3} kg

$\lambda = 10^{-14}$ angstrom, which is too small

For Wave :

$$\psi = \text{A} \sin(\omega t - kx)$$

$\boxed{\text{Phase Velocity } v_p = \frac{\omega}{k} = v\lambda}$

For, mono chromatic yellow-light.

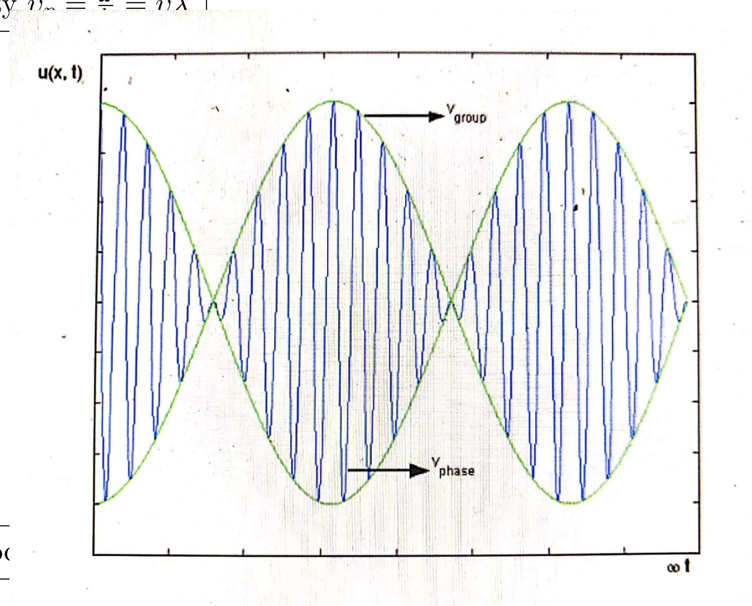
$\psi_1 = \text{A} \sin(\omega t - kx)$

$\psi_2 = \text{A} \sin[(\omega + \Delta\omega)t - (k + \Delta x)x]$

$\rightarrow \psi_{tot} = \psi_1 + \psi_2 = \text{A} \sin(\omega t - kx)$

Resultant:

Amplitude A $= 2\text{a Cos}(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x)$



Group Velo

For Matter Wave :

$$\boxed{v_p = \frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{E}{P}} \text{ and } \boxed{v_g = \frac{d\omega}{dk} = \frac{dE}{dP}}$$

For non-relativistic, $E = \frac{P^2}{2m}$

$\rightarrow v_p = \frac{E}{P} = \frac{P}{2m} = \frac{v}{2} < v < c$

$\rightarrow v_g = \frac{dE}{dP} = \frac{P}{m} = v \Rightarrow$ Group velocity of matter wave=particle velocity

For relativistic, $E = \sqrt{p^2c^2 + m^2c^4}$

$\rightarrow \upsilon_p = \frac{E}{P} = c[1 + \frac{{m_0}^2c^4}{p^2c^2}]^{\frac{1}{2}} > C$

$\rightarrow \upsilon_g = \frac{dE}{dP} = \frac{1}{2}\frac{2pc^2}{[p^2c^2+{m_0}^2c^4]^{\frac{1}{2}}} = \frac{pc^2}{E} = \frac{m\upsilon c^2}{mc^2} = \upsilon$

Here we can see that For relativistic and non-relativistic, the answer is same(υ).

$\upsilon_p = \dfrac{E}{p}$ and $\upsilon_g = \dfrac{pc^2}{E}$ (for relativistic)
$\Rightarrow \upsilon_p\upsilon_g = c^2$

Heisenberg's Uncertainty

In quantum mechanics, the Heisenberg's uncertainty principle is any of a variety of mathematical inequalities, asserting a fundamental limit to the accuracy with which the values for certain pairs of physical quantities of a particle, such as position, x, and momentum, p, can be predicted from initial conditions.
Introduced first in 1927 by the German physicist Werner Heisenberg, **the uncertainty principle states that the more precisely the position of some particle is determined, the less precisely its momentum can be predicted from initial conditions, and vice versa**.

$$\Delta x \Delta P \geq \hbar$$

x and P can't be measured simultaneously with 100% accuracy.

x and P are conjugate variables

$$\begin{aligned}[x][P] &= [L][MLT^{-1}] \\ &= [ML^2T^{-1}]\end{aligned}$$

Similarly, for $\Delta E \Delta t \geq \hbar$, E and t are conjugate variables

$$\begin{aligned}[E][t] &= [FL][T] \\ &= [MLT^{-2}L][T] \\ &= [ML^2T^{-1}]\end{aligned}$$

Chapter 7

Schrodinger's equation(SE) and 1D Potential problem

Time Dependent Schrodinger Equation:

From the observations of the particle in an infinite well,the wave function of a particle of fixed energy E could most naturally be written as a linear combination of wave functions of the form $\psi(x,t) = Ae^{i(kx-\omega t)}$ representing a wave travelling in the positive x direction, and a corresponding wave travelling in the opposite direction, so giving rise to a standing wave, this being necessary in order to satisfy the boundary conditions. This corresponds intuitively to our classical notion of a particle bouncing back and forth between the walls of the potential well, which suggests that we adopt the wave function above as being the appropriate wave function or a free particle of momentum $p = \hbar * k$ and energy $E = \hbar * \omega$.

Now,differentiating the wave function twice gives,

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi$$

since $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$, the equation can be rewritten as:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p^2}{2m}\psi$$

Similarly,

$$\frac{\partial\psi}{\partial t} = -i\omega\psi$$

The above equation can be expressed in terms of energy as $E = \hbar\omega$ as

$$i\hbar\frac{\partial\psi}{\partial t} = \hbar\omega\psi = E\psi$$

The energy term can be written as sum of kinetic energy and potential energy as $E = \frac{p^2}{2m} + V(x)$ then the above equation becomes,

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

Here ψ represents the wave function of a particle moving in the presence of potential field V(x).Rewriting the equation by using energy momentum relation as:

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

This equation is known as **Time Dependent Schrodinger Equation**.

Time Independent Schrodinger Equation:

Now we understand what a wave function looks like for a free particle of energy E, one or the other of the harmonic wave functions and we have seen what it looks like for the particle in an infinitely deep potential well. In both of these cases, the time dependence entered into the wave function via a complex exponential factor $exp[-iEt/\hbar]$.This suggests that to 'extract' this time dependence we guess a solution to the Schrodinger wave equation of the form:

$$\psi(x,t) = \psi(x)e^{-iE\frac{t}{\hbar}}$$

Here, the space and time dependence of the wave function are a separate factors.Substituting this equation into Schrodinger wave equation will give

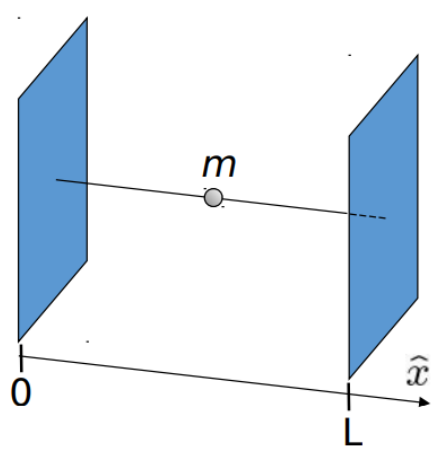
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}e^{-iE\frac{t}{\hbar}} + V(x)\psi(x)e^{-iE\frac{t}{\hbar}} = i\hbar * (-i\frac{E}{\hbar})e^{-iE\frac{t}{\hbar}}\psi(x) = E\psi(x)e^{-iE\frac{t}{\hbar}}$$

The above equation can be rewritten after cancelling the terms as

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

for(x $\leq$ 0 , x $\geq$ L) , V(x) = ∞

$$E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + (\infty)\psi \Rightarrow \psi = 0$$



for(0 < x < L) , V(x) = 0

$$E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \Rightarrow \psi(0) = \psi(L) = 0$$

As wave function must be continuous.

$$E_n\psi_n = -\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2}$$

Rewrite as

$$\frac{\partial^2\psi_n}{\partial x^2} + k_n^2\psi_n = 0 \text{ where, } k_n^2 = \frac{2mE_n}{\hbar^2}$$

The general solution of the above equation is:

$$\psi_n(x) = ASin(k_n x) + BCos(k_n x)$$

Using boundary conditions: $\psi(0) = 0 \Rightarrow$ B = 0 and $\psi(L) = 0 \Rightarrow k_n L = n\pi$.

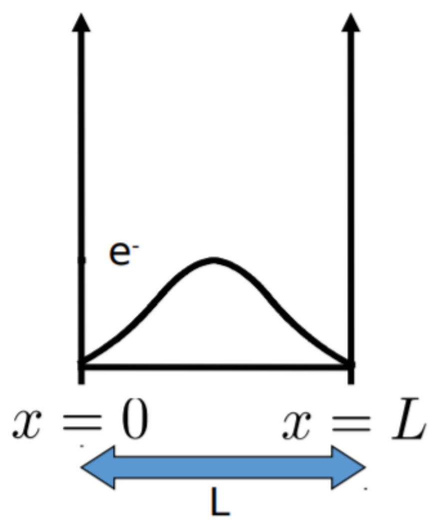
Since,

$$k_n^2 = \frac{2mE_n}{\hbar^2} \Rightarrow E_n = \frac{\hbar^2 k_n^2}{2m}$$
$$k_n = \frac{n\pi}{L} \Rightarrow E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}$$

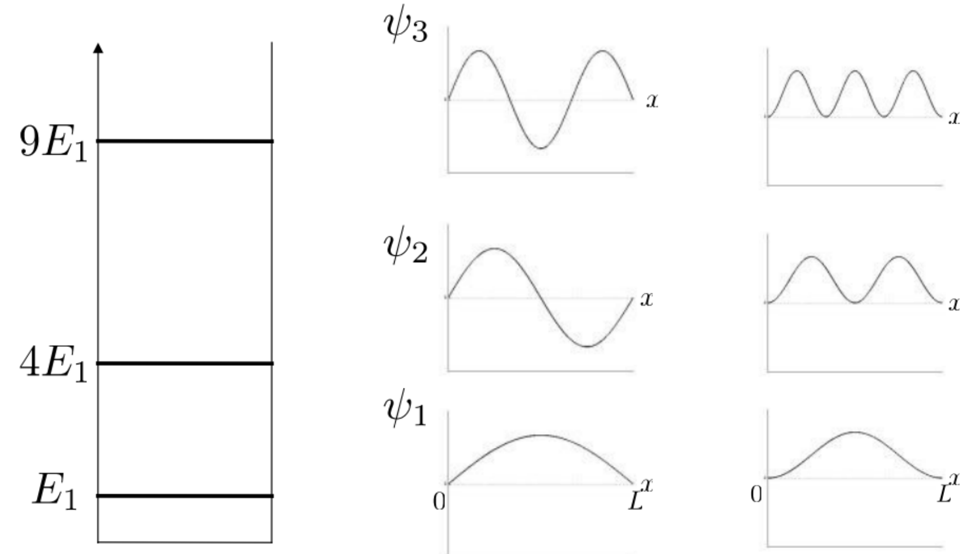
As $E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2\pi^2}{2mL^2} \Rightarrow E_n = n^2 E_1$.
Here, E_n indicates the energy of n^{th} state.

Normalizing the wave function to probability of 1 gives,

$$\psi_n(x) = \sqrt{\frac{2}{L}} Sin\frac{n\pi x}{L}$$



The wave function $\psi_n(x)$ indicates the n_{th} eigen state.This result can be represented graphically for a particle in a 1-D Box.



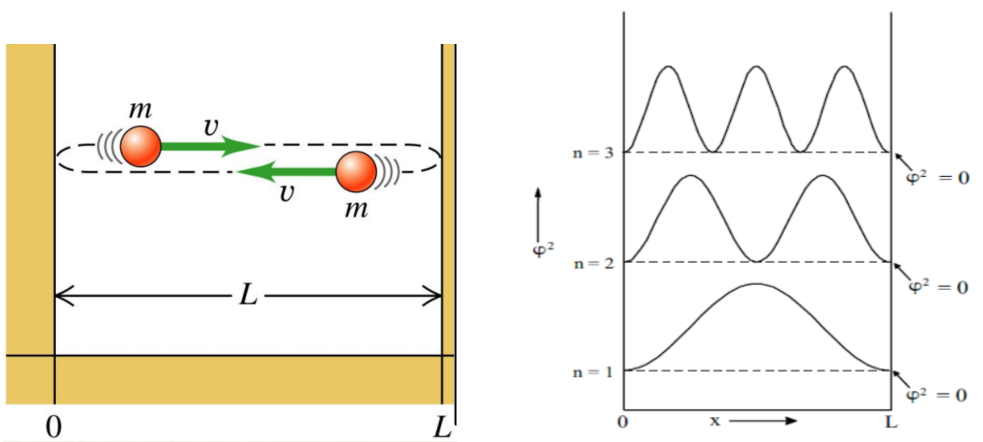
(a) Eigen Energies for 1-D Box

(b) Eigen states for 1-D Box

(c) Probability Densities

Probability Density $P(x) = |\psi(x)|^2 dx = \frac{2}{L} sin^2 \frac{n\pi x}{L} dx$.

The difference in the outcomes of classical and quantum view is shown below:



(a) Classical View-Definite Existence in Space

(b) Quantum View-Probabilistic Existence in Space

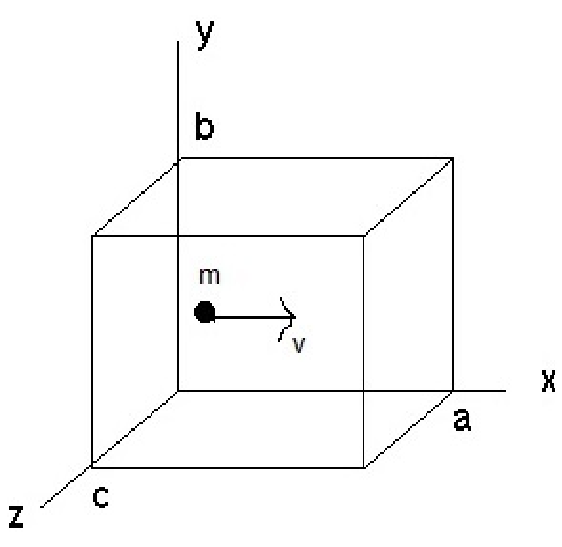
Chapter 8

Potential problems

gross message from materials from LecSE2 ppt (12 slides) and potential problem notes (page 1-4)

8.1 Particle in 3-D Box

$$V(x,y,z) = \begin{cases} 0 & \text{if; } 0 < x < a, 0 < y < b, 0 < z < c \\ \infty & ;otherwise \end{cases}$$



wave function of particle:

$$\Psi(x,y,z) = \psi(x)\psi(y)\psi(z)$$
$$\Psi(x,y,z) = \sqrt{\frac{2}{a}}\sin\frac{n_x\pi x}{a}\sqrt{\frac{2}{b}}\sin\frac{n_y\pi y}{b}\sqrt{\frac{2}{c}}\sin\frac{n_z\pi z}{c}$$
$$\Psi(x,y,z) = \sqrt{\frac{8}{abc}}\sin\frac{n_x\pi x}{a}\sin\frac{n_y\pi y}{b}\sin\frac{n_z\pi z}{c}$$

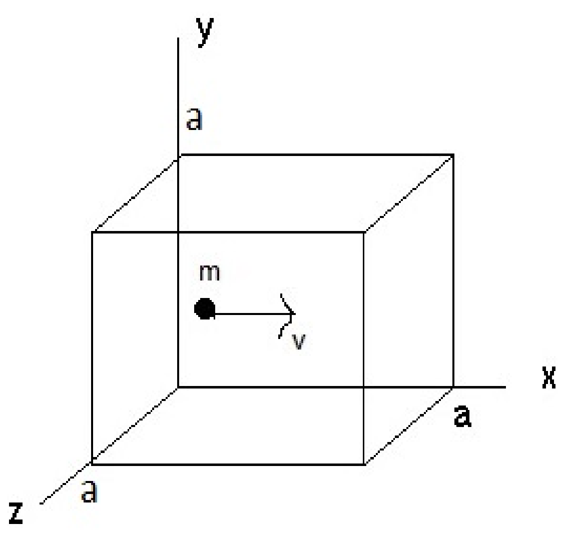
Energy eigen value of particle

$$E = \frac{n_x^2\pi^2\hbar^2}{2ma^2} + \frac{n_y^2\pi^2\hbar^2}{2mb^2} + \frac{n_z^2\pi^2\hbar^2}{2mc^2}$$

The integers n_x, n_y, n_z are quantum numbers which are required to describe the stationary state of particle.Always n_x, n_y, n_zan integer and start from 1 i.e. $n_x = 1, 2, ...$, $n_x = 1, 2, ...$, $n_x = 1, 2, ...$

8.2 Particle in 3-D Cubical Box

$$V(x,y,z) = \begin{cases} 0 & \text{if}; 0 < x < a, 0 < y < a, 0 < z < a \\ \infty & ;otherwise \end{cases}$$



wave function of particle:

$$\Psi(x,y,z) = \psi(x)\psi(y)\psi(z)$$
$$\Psi(x,y,z) = \sqrt{\frac{2}{a}}\sin\frac{n_x\pi x}{a}\sqrt{\frac{2}{a}}\sin\frac{n_y\pi y}{a}\sqrt{\frac{2}{a}}\sin\frac{n_z\pi z}{a}$$
$$\Psi(x,y,z) = \sqrt{\frac{8}{a^3}}\sin\frac{n_x\pi x}{a}\sin\frac{n_y\pi y}{a}\sin\frac{n_z\pi z}{a}$$

Energy eigen value of particle

$$E = \frac{n_x^2\pi^2\hbar^2}{2ma^2} + \frac{n_y^2\pi^2\hbar^2}{2ma^2} + \frac{n_z^2\pi^2\hbar^2}{2ma^2}$$
$$E = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

Degeneracy

The property that,two or more quantum states of a particle,with different sets of quantum numbers and different eigenfunctions having the same value of momentum and energy is called degeneracy. For example,the three states of corresponding to quantum numbers (2,1,1) ,(1,2,1),(1,1,2) all have the same momentum $\left(\frac{\pi\hbar}{a}\sqrt{6}\right)$ and energy $\left(\frac{\pi^2\hbar^2}{2ma^2}6\right)$ so here degeneracy is 3.

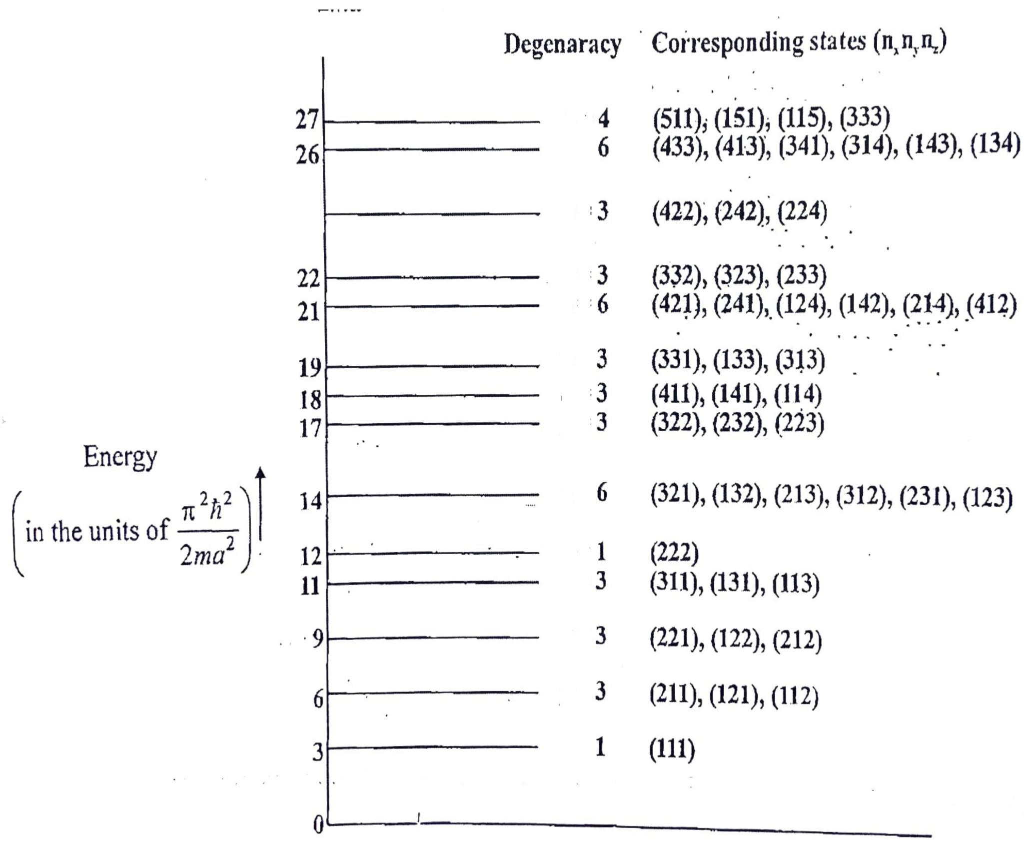


Figure : Energy levels of a particle in a cubical potential box

Potential problem

Here we will discuss what happens when a beam of particles of fixed energy is incident on a potential barrier.Classically there must be complete transmission if energy of incident particle is more than height of barrier and total reflection if energy is less than the height of the barrier.

let's do the quantum mechanical treatment of same first by considering step potential and then by potential barrier problem

8.3 step potential

Let us consider the potential step as shown in figure. It is an infinite width potential barrier given by

$$V(x) = 0 \qquad x < 0$$
$$V(x) = V_0 \qquad x \geq 0$$

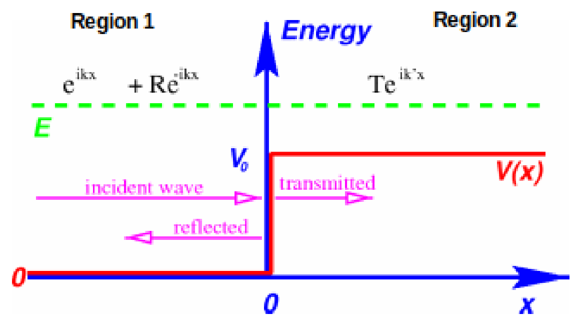


Figure 8.1: the potential step

Let a particle is incident on the step from left with energy E.there will be two cases$E < V_0$ and $E > V_0$.First we will consider $E > V_O$ case. Classically particle should transmit without reflection.
Let's check from quantum mechanical treatment of $E > V_0$ **case** let's start from time independent schrodinger's equation as particle motion is independent of time.
In **region** 1 $x < 0, V(x) = 0$ the schrodinger's equation is

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

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \qquad k^2 = \frac{2mE}{\hbar^2}$$

the solution of this equation is

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

The term Ae^{ikx} corresponds to incident wave and term Be^{-ikx} corresponds to reflected wave from step.So,according to quantum mechanics the particle may be reflected back at $x = 0$ for $E > V_0$.This is not possible classically.
In **region 2** $x > 0$,$V(x) = V_0$ schrodinger's equation is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} + k_1^2\psi(x) = 0, \qquad k_1 = \frac{2m(E-V_0)}{\hbar^2}$$

the general solution is

$$\psi(x) = Ce^{ik_1x} + De^{-ik_1x}$$

in region 2 there is nothing to reflect,so D must be = 0

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad x < 0 \tag{8.1}$$

$$= Ce^{ik_1x} \qquad x > 0 \tag{8.2}$$

from continuity of $\psi(x)$ and$\frac{d\psi(x)}{dx}$ at $x = 0$ gives

$$A + B = C$$

$$k(A - B) = k_1C$$

after solving we get

$$\frac{B}{A} = \frac{k-k_1}{k+k_1}$$

and

$$\frac{C}{A} = \frac{2k}{k+k_1}$$

A particle incident will be reflected or transmitted.The probability of reflection is given by reflection coefficient R.

$$R = \frac{\frac{\hbar k}{m}|B^2|}{\frac{\hbar k}{m}|A^2|} = \frac{|B^2|}{|A^2|} = \frac{k-k_1}{k+k_1}$$

after putting kalue of k and k_1

$$R = \left[\frac{1-(1-\frac{V_0}{E})^{1/2}}{1+(1-\frac{V_0}{E})^{1/2}}\right]^2 \qquad E > V_0$$

The probability of transmission is given by transmission coefficient T

$$T = \frac{k_1|C|^2}{k|A|^2} = \frac{4kk_1}{(k+k_1)^2}$$

after putting values of k_1 and k

$$T = \frac{4(1-\frac{V_0}{E})^{1/2}}{[1+(1-\frac{V_0}{E})^{1/2}]^2} \qquad E > V_0$$

Note that $R + T = 1$ must be followed as probability is conserved
The only thing we get from above calculaions that for $E > V_0$ reflection can be possible which was not the case classically.
Now we will do the calculations for $E < V_0$ case and check what new information or phenomenon we can get from there.

$E < V_0$ case

Cosider a beam of particales each of mass m and energy E moving alog x-axis from left to right on the following potential:
$V(x) = 0$ for $x < 0$ Region 1
$V(x) = V_0$ for $x > 0$ Region 2

Rgion 1
The potential

$$V(x) = 0. \tag{8.3}$$

$E > V(x)$therefore

$$\psi_1 = Aexp(ik_2x) + Bexp(-ik_1x)(x < 0) \tag{8.4}$$

here $k_1 = k$ from previous case of $E > V$,it should not be confused with a new constant
Region-2
The potential $V(x) = V_0$. since $E < V(x)$
therefore

$$\psi_2 = Cexp(k_2x) + Dexp(-k_2x)(x > 0)$$

$$\psi_2(x = infinite) = infinite$$

i.e.

$$C = 0$$

$$\psi_2 = Dexp(-k_2x)$$

here k_2 is a new constant
$k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(V_0 - E)/\hbar^2$
According to classical theory , if the energy of the particle is less than the height of the potential step i.e. $E < V_0$. then particle cannot penetrate into Region-2. All particles will be reflected back into the Region-1 from the boundary at x=0. therefore,Region-2 is classically forbidden region.

According to Quantum theory,if the energy of the of the particle is less than the height of the potential step $E < V$
then particles can be penetrate into region -2 .since ,there is a wave nature associated with a moving particle ,therefore the position of the boundary from which particles reflect back into region-1 is also uncertain.Maximum number of particle will be reflected back from x=0 and remaining number of particles will be reflected back after penetrating up to a certain distance into classically forbidden region.

Penetration Depth (d)

The phenomena of particle getting into classically forbidden region is "Barrier Penetration".In the classically forbidden region ,the wave function of the particle decays exponentially with a length scale of 'd'. This means,the magnitude of the wave function becomes negligible at a distance of few times of "d".
At x=d, the value of the wave function becomes 1/e times of it's value at the boundary (x=0)

$$d = 1/k_2 = \hbar/\sqrt{(}2m(V_0 - E)) \tag{8.5}$$

Evaluation of constants A,B and D

Boundary Condition-1
ψ should be continuous at $x = 0$ i.e.

$$\psi_1(x = 0) = \psi_2(x = 0) \qquad A + B = D \tag{8.6}$$

Boundary Condition 2
$d\psi/dx$ should be continuous at $x = 0$i.e.

$$d\psi_1/dx(x = 0) = d\psi_2/dx(x = 0) \qquad A - B = ik_2/k_1 D \tag{8.7}$$

using above equations,we can obtain
$B = (k_1 - ik_2)A/(k_1 + ik_2)$
$D = 2k_1 A/(k_1 + ik_2)$

Reflection and Transmission Co-efficient

R=Number of reflected particles/Number of incident particles
= Reflected flux/Incident flux

$$= J_r ef/J_i nc \tag{8.8}$$

T= Number of transmitted particles/number of incident particles
=Transmitted Flux/Incident Flux
$= J_{tra}/J_{inc}$
Reflection Coefficient(probability of Reflection) is defined as
$R = J_{ref}/J_{inc}$

$\hbar k_1|B|^2/m]/[\hbar k_1|A|^2/m$
here$A = B$
$= 1$ (100 percent Reflection)
Transmission Co-efficient(Probability of Transmission) is defined as

$$T = J_{tra}/J_{inc}$$

$$= [0]/[\hbar k_1|A|^2/m]$$

$$= 0$$

This result shows that there is finite probability of finding the particle in classicaly forbidden region 2 ,there is no permanent penetration . It means that there is continuous reflection in region 2 until all the incident particles are returned to region 1.

Chapter 9

Square potential barrier:

We now consider a one-dimensional potential barrier of finite width and height given by

$$V(x) = 0 \qquad x < 0$$

$$V(x) = V_0 \qquad 0 < x < a$$

$$V(x) = 0 \qquad x > a$$

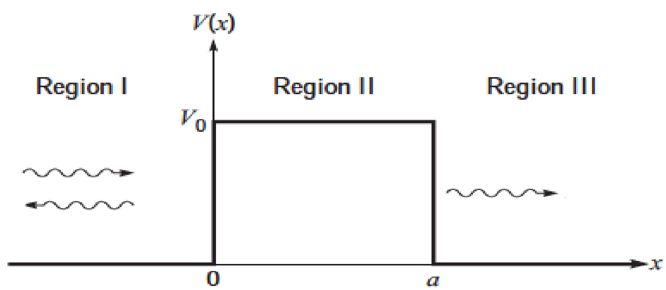


Figure 9.1: The square potential barrier

Such a barrier is called a square or a rectangular barrier and is shown in figure above.
We consider a particle of mass m incident on the barrier from the left with energy E. According to classical mechanics, the particle would always be reflected back if $E < V_0$.

Case : $E < V_0$

Let us divide the whole space into three regions: Region I ($x < 0$), Region II ($0 < x < a$) and Region III ($x > a$). In regions I and III the particle is free and so the time-independent Schrödinger equation is

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

or

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \qquad k^2 = \frac{2mE}{\hbar^2}$$

The general solution of this equation is

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad x < 0$$

$$\psi(x) = Fe^{ikx} + Ge^{-ikx} \qquad x > a$$

where A, B, F, G are arbitrary constants. For $x < 0$, the term Aexp(ikx) corresponds to a plane wave of amplitude A incident on the barrier from the left and the term Bexp(–ikx) corresponds to a plane wave of amplitude B reflected from the barrier. For $x > a$, the term Fexp(ikx) corresponds to a transmitted wave of amplitude F. Since no reflected wave is possible in this region we must set G=0.
In region II the Schrödinger equation is,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi = E\psi$$

or

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi(x) = 0, \qquad \alpha^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

Since $E < V_0$, the quantity α^2 is positive. Therefore, the general solution of this equation is,

$$\psi(x) = Ce^{-\alpha x} + De^{\alpha x} \qquad 0 < x < a$$

The complete eigenfunction is given by,

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx} \qquad x < 0$$

$$\psi_2(x) = Ce^{-\alpha x} + De^{\alpha x} \qquad 0 < x < a$$

$$\psi_3(x) = Fe^{ikx} \qquad x > a$$

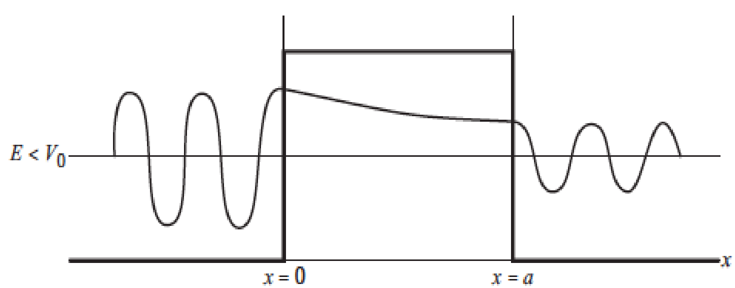


Figure 9.2: Schematic plot of the real part of the barrier eigenfunctions for $E < V_0$

Boundary conditions:

$$\psi_1(0) = \psi_2(0)$$

$$\left(\frac{\partial\psi_1}{\partial x}\right)_{x=0} = \left(\frac{\partial\psi_2}{\partial x}\right)_{x=0}$$

$$\psi_2(a) = \psi_3(a)$$

$$(\frac{\partial \psi_2}{\partial x})_{x=a} = (\frac{\partial \psi_3}{\partial x})_{x=a}$$

Transmission coefficient is given as,

$$T = |\frac{F}{A}|^2 \approx \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)} \sinh^2 \frac{\sqrt{2m(V_0-E)}a}{\hbar}}$$

Now, we solve the following eigenfunctions,

$$\psi_1 = e^{ikx} + Ae^{-ikx}$$

$$\psi_2 = Be^{\alpha x} + Ce^{-\alpha x}$$

$$\psi_3 = De^{ikx}$$

Using the boundary conditions,

(a) $\psi_1(0) = \psi_2(0)$

$$1 + A = B + C \tag{9.1}$$

(b) $(\frac{\partial \psi_1}{\partial x})_{x=0} = (\frac{\partial \psi_2}{\partial x})_{x=0}$

$$ik - ikA = \alpha B - \alpha C \tag{9.2}$$

(c) $\psi_2(a) = \psi_3(a)$

$$Be^{\alpha a} + Ce^{-\alpha a} = De^{ika} \tag{9.3}$$

(d) $(\frac{\partial \psi_2}{\partial x})_{x=a} = (\frac{\partial \psi_3}{\partial x})_{x=a}$

$$\alpha Be^{\alpha a} - \alpha Ce^{-\alpha a} = ikDe^{ika} \tag{9.4}$$

Now, on multiplying equation 9.3 by α and adding equation 9.4 to it, we get,

$$2\alpha Be^{\alpha a} = (\alpha + ik)De^{ika} \tag{9.5}$$

$$B = \frac{D}{2\alpha}(\alpha + ik)e^{ika-\alpha a} \tag{9.6}$$

Now, on multiplying equation 9.3 by α and subtracting equation 9.4 from it, we get,

$$2\alpha Ce^{-\alpha a} = (\alpha - ik)De^{ika} \tag{9.7}$$

$$C = \frac{D}{2\alpha}(\alpha - ik)e^{ika+\alpha a} \tag{9.8}$$

Put the value of A from equation 9.1 into equation 9.2,

$$ik - ik(B + C - 1) = \alpha B - \alpha C \tag{9.9}$$

$$2ik = (\alpha + ik)B + (-\alpha + ik)C \tag{9.10}$$

Substituting the values of B and C in equation 9.10, we get,

$$\frac{D}{2\alpha}e^{ika}\Big\{(\alpha + ik)^2 - (\alpha - ik)^2 e^{\alpha a}\Big\} = 2ik$$

$$D = \frac{2ik\alpha e^{-ika}}{(\alpha^2 - k^2)\sinh(\alpha a) + 2ik\alpha\cosh(\alpha a)} \tag{9.11}$$

Using equation 9.11, we find the value of transmission coefficient,

$$T = |D|^2$$

$$T = \frac{4k^2\alpha^2}{(\alpha^2 - k^2)^2\sinh^2(\alpha a) + 4\alpha^2k^2\cosh^2(\alpha a)}$$

For a broad (large value of a) and high (large value of V_0) barrier,

$$\alpha a = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}a >> 1 \qquad (\sinh(\alpha a) \approx \cosh(\alpha a) \approx \frac{e^{\alpha a}}{2})$$

$$T = \frac{4k^2\alpha^2}{\Big\{(\alpha^2 - k^2)^2 + 4\alpha^2k^2\Big\}\frac{e^{2\alpha a}}{4}}$$

$$T = \frac{16k^2\alpha^2e^{-2\alpha}}{(\alpha^2 + k^2)^2} \tag{9.12}$$

Substituting the value of α in equation 9.12, we get,

$$T = \frac{16(V_0 - E)e^{-2\alpha a}}{V_0^2} \tag{9.13}$$

where $\alpha = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

Chapter 10

Quantum Postulates

materials from Quantum Postulates notes (page 1-2)

Commutation relation → Simultanous measurement → possiblle → not-possible

$$[\hat{O}_1, \hat{O}_2]|\psi\rangle = [\hat{O}_1\hat{O}_2 - \hat{O}_2\hat{O}_1]|\psi\rangle = 0 \text{ (zero)}$$
$$\neq 0$$

Example

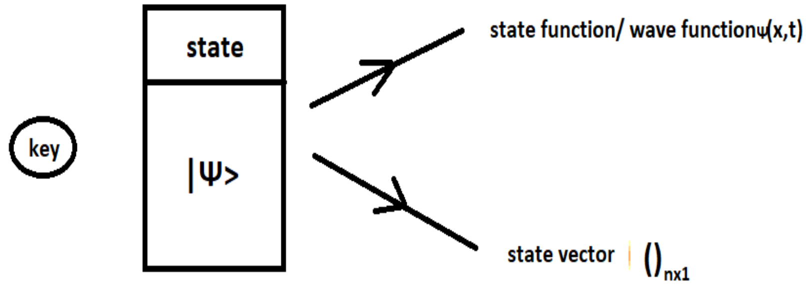
$$[\hat{x}, \hat{P}_y] = [\hat{x}, \hat{P}_z] = [\hat{y}, \hat{P}_x] = [\hat{y}, \hat{P}_z] = [\hat{z}, \hat{P}_x] = [\hat{z}, \hat{P}_y] = 0$$

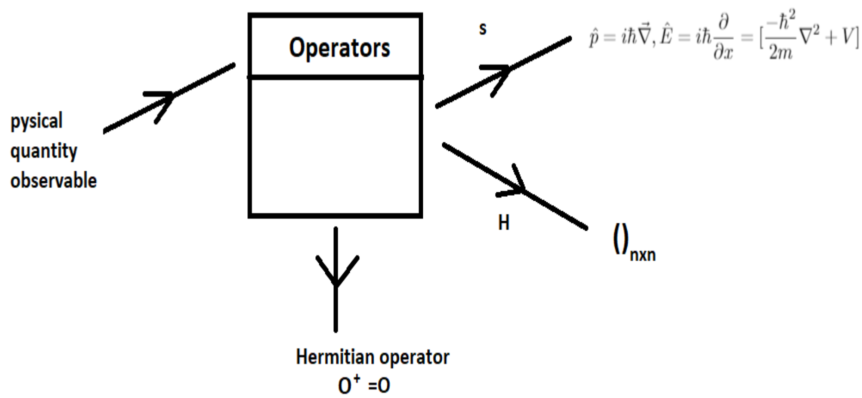
but $[\hat{x}, \hat{P}_x] = [\hat{y}, \hat{P}_y] = [\hat{z}, \hat{P}_z] = i\hbar \neq 0$

Check

$$\begin{aligned}
[\hat{x}, \hat{P}_x]|\psi\rangle &= (\hat{x}\ \hat{P}_x - \hat{P}_x\ \hat{x})|\psi\rangle \\
&= x\Big(-i\hbar\frac{\partial}{\partial x}\Big)\psi - \Big(-i\hbar\frac{\partial}{\partial x}\Big)(x\psi) \\
&= -i\hbar\Big(x\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial x} - \psi\frac{\partial x}{\partial x}\Big)
\end{aligned}$$

$$[\hat{x}, \hat{P}_x]|\psi\rangle = i\hbar|\psi\rangle \Rightarrow [\hat{x}, \hat{P}_x] = i\hbar$$





10.1 Postulate-1

10.2 Postulate-2

Angular momentum operator

$$L = \vec{r} X \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ -ih\frac{\partial}{\partial x} & -h\frac{\partial}{\partial y} & -ih\frac{\partial}{\partial z} \end{vmatrix} = L_x\hat{i} + L_y\hat{j} + L_z\hat{k}$$

Commutation relation → Simultanous measurement → possiblle → not-possible

$$[\hat{O}_1, \hat{O}_2]|\psi\rangle = [\hat{O}_1\hat{O}_2 - \hat{O}_2\hat{O}_1]|\psi\rangle = 0 \text{ (zero)}$$
$$\neq 0$$

e.g

$$[\hat{x}, \hat{P}_y] = [\hat{x}, \hat{P}_z] = [\hat{y}, \hat{P}_x] = [\hat{y}, \hat{P}_z] = [\hat{z}, \hat{P}_y] = [\hat{z}, \hat{P}_x] = 0$$

but

$$[\hat{x}, \hat{P}_x] = [\hat{y}, \hat{P}_y] = [\hat{z}, \hat{P}_z] = i\hbar \neq 0$$

Check

$$\begin{aligned}
[\hat{x}, \hat{P}_x]|\psi\rangle &= (\hat{x}\ \hat{P}_x - \hat{P}_x\ \hat{x})|\psi\rangle \\
&= x\Big(-i\hbar\frac{\partial}{\partial x}\Big)\psi - \Big(-i\hbar\frac{\partial}{\partial x}\Big)(x\psi) \\
&= -i\hbar\Big(x\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial x} - \psi\frac{\partial x}{\partial x}\Big) \\
[\hat{x}, \hat{P}_x]|\psi\rangle &= i\hbar|\psi\rangle \Rightarrow [\hat{x}, \hat{P}_x] = i\hbar
\end{aligned}$$

Postulate-3

Expectation value $\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle$

for any ket $|\psi\rangle$ and bra $\langle\psi|$

$\langle\psi \mid \psi\rangle = |\psi(x,t)|^2 S$

probability density=$\begin{pmatrix} o & o & o & . & . & . \end{pmatrix}_{1\times n} \begin{pmatrix} o \\ o \\ o \\ . \\ . \\ . \end{pmatrix}_{n\times 1}$

probability density=$o^2 + o^2 + ...$

Postulate-4:-

Eigen value $\hat{O}|\psi\rangle = \lambda_0|\psi\rangle$
$\hat{O}$: operator
λ_0 : Eigen value
$|\psi\rangle$: Eigen vector/function

Ex. 1D box, $\hat{O} \equiv \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

$|\psi\rangle \equiv \psi(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)e^{iEt/\hbar}$

$\hat{O}|\psi\rangle \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left\{\sqrt{\frac{2}{L}}\sin\left(\frac{n^2}{L}x\right)e^{iEt/\hbar}\right\}$

$= +\frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2\left\{\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)e^{iEt}\right\} = \left(\frac{\hbar^2\pi^2}{2mL^2}\right)n^2\psi(x,t)$

$\hat{H}|\psi\rangle = \lambda_E|\psi\rangle \Rightarrow \lambda_E = E_n = \left(\frac{\hbar^2\pi^2}{2mL^2}\right)n^2 \Rightarrow$ Energy Eigen Value

Postulate-5 - Time evolution of Quantum system

$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t)$

10.3 Quick revisit of Classical Harmonic Oscillator (CHO) and entering into quantum harmonic oscillator (QHO)

We know

$$V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$$

From Classical Mechanics

$$\ddot{x} + \omega^2x = 0$$

According to Langrangian

$$\dot{L} = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$$

$$\frac{\partial L}{\partial x} = \frac{\partial(\frac{\partial L}{\partial \dot{x}})}{\partial t}$$

According to Newtonian

$$m\ddot{x} = -kx$$

Now

$$x = aSin\omega t$$

$$E_K = \frac{1}{2}m\dot{x}^2 = \frac{1}{2}m\omega^2a^2Cos^2\omega t$$

$$V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2a^2Sin^2\omega t$$

$$E_t = \frac{1}{2}m\omega^2a, ClassicalMechanics$$

$$E_t = (n + \frac{1}{2})\hbar\omega, QuantumMechanics$$

As ω increases $k = m\omega$ increase and E_t increases
As a increases E_t increases
From Quantum machanics:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2\psi = E\psi$$

Putting $k = x^2$

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

From $y = \sqrt{\frac{m\omega}{\hbar}}$

$$\frac{-\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{\partial^2\psi}{\delta y^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi$$

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

Multiply bith side with $\frac{-2m}{\hbar^2}$

$$\frac{\partial^2\psi}{\partial y^2} - \frac{m^2\omega^2x^2}{\hbar^2\psi} = \frac{-2mE\psi}{\hbar^2}$$

$$\frac{\partial^2\psi}{\partial y^2} + \frac{2mE\psi}{\hbar^2} - \frac{m^2\omega^2x^2}{\hbar^2\psi} = 0$$

$$\frac{\partial^2\psi}{\partial y^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2x^2}{\hbar^2}\right)\psi = 0$$

$$\frac{\partial^2\psi}{\partial y^2} + \left(\frac{2E}{\hbar\omega} - \frac{m\omega x^2}{\hbar}\right)\psi = 0$$

$$\frac{\partial^2\psi}{\partial y^2} + \left(\lambda - y^2\right)\psi = 0$$

Where $\lambda = \frac{2E}{\hbar\omega}$ and $y^2 = \frac{m\omega}{\hbar}$

Asymptotic solution at $y \to \alpha$, where $\lambda - y^2 \cong -y^2$

$$\frac{\partial^2\psi}{\partial y^2} - y^2\psi = 0$$

$$\psi(y) = e^{\pm\frac{y^2}{2}}$$

$$\frac{\partial^2\psi}{\partial y^2} = (y^2+1)e^{\pm\frac{y^2}{2}} \approx y^2e^{\pm\frac{y^2}{2}}$$

$e^{+\frac{y^2}{2}}$ is not-well behaved function
Now $\psi = e^{-\frac{y^2}{2}}$ which is Asymptotic.

Guess exact solution:

$$\psi(y) = e^{-\frac{y^2}{2}} H(y)$$

such that $\psi(y = \alpha) = 0$

$$\frac{\partial^2 H(y)}{\partial y^2} - 2y\frac{\partial H(y)}{\partial y} + (\lambda - 1)H(y) = 0$$

This is a well known Hermite equation

$$H(y) = \sum_{n=0}^{\infty} a_n y^n$$

Equating coefficient of y^n (for any value of n), we get the following recurrence relation:

$$a_{n+2} = \frac{2n + 1 - \lambda}{(n + 1)(n + 2)} a_n$$

$$H_{even} = a_0 + a_2 y^2 + a_4 y^4 + ...$$
$$H_{odd} = y(a_1 + a_3 y^2 + a_5 y^4 + ...)$$

Terminating series condition

$$2n + 1 - \lambda = 0$$
$$\Rightarrow \lambda = 2n + 1$$
$$\frac{2E_n}{\hbar\omega} = (2n + 1)$$
$$\Rightarrow E_n = (n + \frac{1}{2})\hbar\omega$$

Chapter 11

On Solution of quantum harmonic oscillator (QHO)

Quantum harmonic oscillator: The quantum harmonic oscillator is the quantum-mechanical analog of the classical harmonic oscillator. Because an arbitrary smooth potential can usually be approximated as a harmonic potential at the vicinity of a stable equilibrium point, it is one of the most important model systems in quantum mechanics.

So for $\lambda = 2n + 1$

Hermite equation becomes

$\frac{\partial^2}{\partial x_2^2} H_n(y) - 2y \frac{\partial H_n(y)}{\partial y} + 2nH_n(y) = 0$

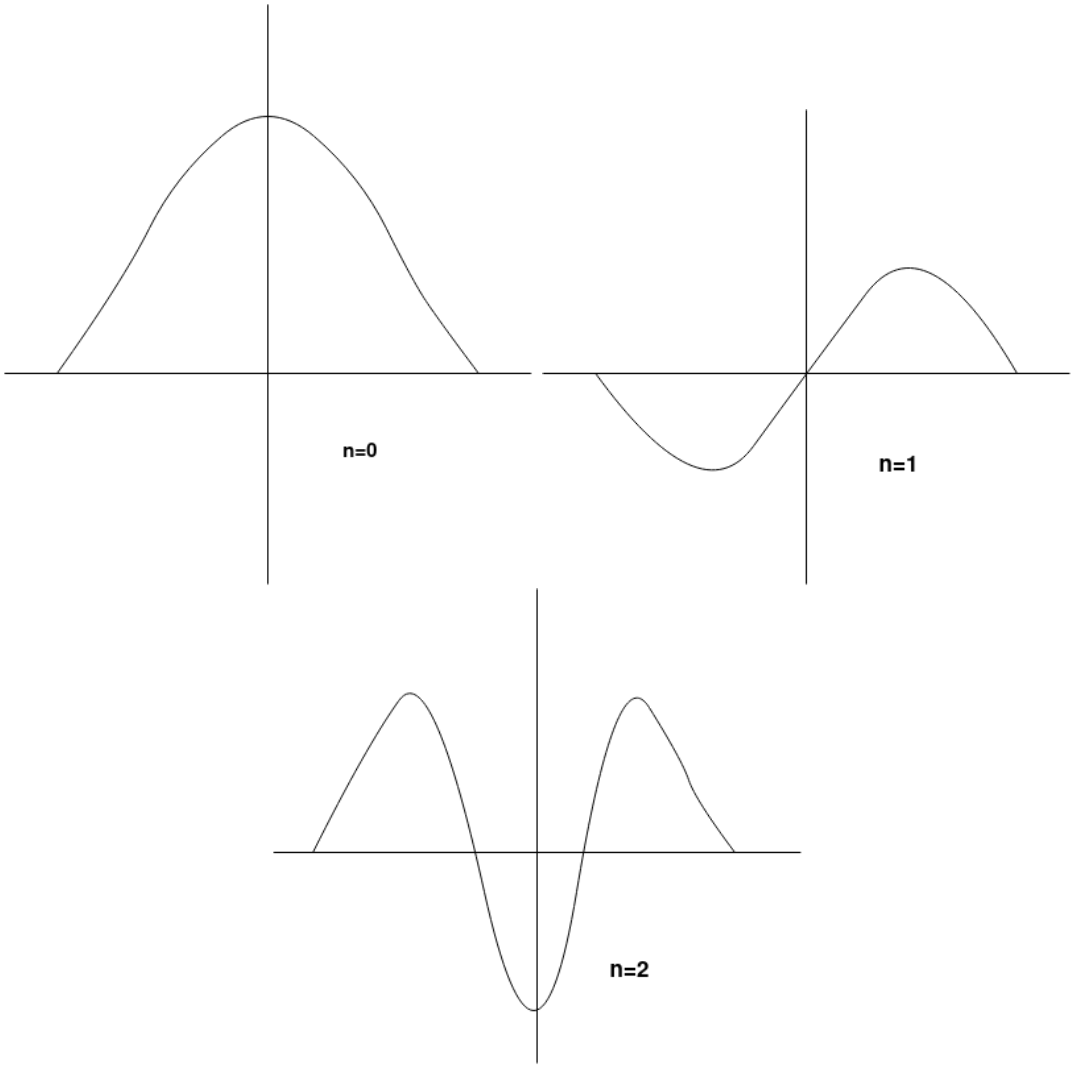
$\Rightarrow \psi_n(y) = N_n H_n(y) e^{\frac{-y^2}{2}}$ where H_n is hermite polynomial.
Hermite polynomial for n=0,1,2

$H_0(y) = 1$

$H_1(y) = 2y$

$H_2(y) = 4y^2 - 2$

$H_3(y) = 8y^3 - 12y$



$V(x) = \frac{1}{2}m\omega^2 x^2$
$x \uparrow \Rightarrow V(x) \uparrow$

$\frac{1}{2}\hbar\omega = \frac{1}{2}m\omega^2 a^2$

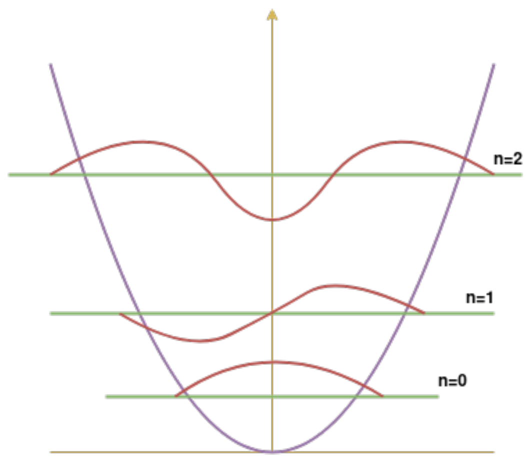
$\langle V \rangle = \int \psi' v(\alpha)\psi$

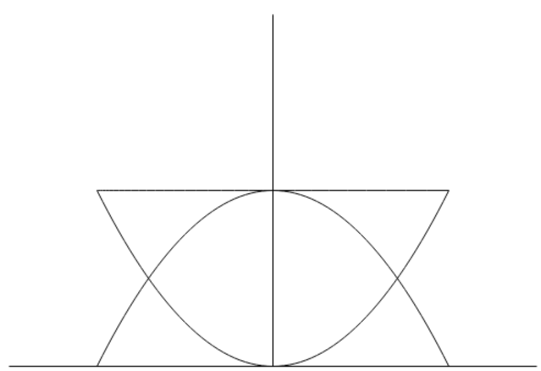
$= |N|^2 \int_0^\infty e^{-\frac{2m\omega x^2}{2\hbar}} \frac{1}{2}m\omega^2 x^2$
$= \left(\frac{m\omega}{\hbar?}\right)^{\frac{1}{2}} m\omega^2 \int_0^\infty e^{-m\omega x^2/\hbar} \cdot x^2 dx$

$\frac{m\omega x^2}{\hbar} = z$
$\frac{m\omega}{\hbar} 2x dx = dz$ $\langle V \rangle = \left(\frac{m\omega}{\hbar?}\right)^{1/2} \int_0^\infty e^{-z} m\omega^2 \frac{\hbar}{2m\omega} dz \left(\frac{\hbar z}{m\omega}\right)^{\frac{1}{2}}$

$= \left(\frac{m\omega}{\hbar?}\right)^{\frac{1}{2}} \cdot \frac{\hbar}{2} \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}} \Gamma\left(\frac{3}{2}\right)$

$\Gamma(\frac{3}{2}) = \frac{1\sqrt{\hbar}}{2}$


n=2
n=1
n=0



Chapter 12

Operator methods of quantum harmonic oscillator (QHO)

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12.1 Operator Method

By using of operator method we get energy eigenvalue of linear harmonic oscillator.And below is some new things which will be useful to get energy eigenvalue.
(a). Annihilation Operator

$$\hat{a} = A\hat{x} + \iota B\hat{p}$$

It is also known as **lowering operator** because when it operates on a $|n\rangle$ state then we get a new state which is $|n-1\rangle$, means lower state to given state.

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$

(b).Creation Operator

$$\hat{a}^\dagger = A\hat{x} - \iota B\hat{p}$$

It is also known as **raising operator** because when it operates on a $|n\rangle$ state then we get a new state which is $|n+1\rangle$, means higher state to given state.

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

where $\hat{a}$ and $\hat{a}^\dagger$ is hermition cojugate and

$$A = \sqrt{\frac{m\omega}{2\hbar}}$$

and

$$B = \sqrt{\frac{1}{2m\hbar\omega}}$$

(c).Number Operator

$$N = \hat{a}^\dagger \hat{a}$$

When it operates on a state$|n\rangle$ then we get same state.

$$N|n\rangle = \hat{a}^\dagger \hat{a}|n\rangle = n|n\rangle$$

and we know Hamiltonian operator for linear harmonic oscillator is

$$\hat{H} = \frac{1}{2}m\omega\hat{x}^2 + \frac{\hat{p}^2}{2m}$$

Here $\hat{x}$ is position operator and $\hat{p}$ is momentum operator.
now we calculate $\hat{a}\hat{a}^\dagger$

$$\hat{a}\hat{a}^\dagger = A^2\hat{x}^2 + B^2\hat{p}^2 + \iota AB\left(\hat{p}\hat{x} - \hat{x}\hat{p}\right) \tag{12.1}$$

on putting value of A and B

$$\hat{a}\hat{a}^\dagger = \frac{m\omega}{2\hbar}\hat{x}^2 + \frac{1}{2m\hbar\omega}\hat{p}^2 + \frac{\iota}{2\hbar}\left(\hat{p}\hat{x} - \hat{x}\hat{p}\right)$$

We know that

$$\left(\hat{p}\hat{x} - \hat{x}\hat{p}\right) = [\hat{p}, \hat{x}] = -\iota\hbar$$

and

$$\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right) = [\hat{x}, \hat{p}] = \iota\hbar$$

now using equation (77)

$$\hat{a}\hat{a}^\dagger = A^2\hat{x}^2 + B^2\hat{p}^2 + \hbar AB \tag{12.2}$$

$$= \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \tag{12.3}$$

similarly we can find $\hat{a}^\dagger\hat{a}$

$$\hat{a}^\dagger\hat{a} = A^2\hat{x}^2 + B^2\hat{p}^2 + \iota AB\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)$$

$$\hat{a}^\dagger\hat{a} = A^2\hat{x}^2 + B^2\hat{p}^2 - \hbar AB \tag{12.4}$$

$$= \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \tag{12.5}$$

Now we will find comutator of $\hat{a}$ and $\hat{a}^\dagger$

$$\left[\hat{a}, \hat{a}^\dagger\right] =??$$

$$\left[\hat{a}, \hat{a}^\dagger\right] = \left(\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\right)$$

now using equation (78) and (80) on putting value of $\hat{a}\hat{a}^\dagger$ and $\hat{a}^\dagger\hat{a}$,we get

$$\left[\hat{a}, \hat{a}^\dagger\right] = 2\hbar AB$$

after put the value of A and B ,we get

$$\boxed{\left[\hat{a}, \hat{a}^\dagger\right] = 1}$$

A new thing we will see here that is

$$A^2\hat{x}^2 + B^2\hat{p}^2 = ??$$

when we put the value of A and B in above form,we get

$$\frac{m\omega}{2\hbar}\hat{x}^2 + \frac{1}{2m\hbar\omega}\hat{p}^2 = \frac{1}{\hbar\omega}\left(\frac{1}{2}m\omega\hat{x}^2 + \frac{\hat{p}^2}{2m}\right)$$

$$\boxed{A^2\hat{x}^2 + B^2\hat{p}^2 = \frac{\hat{H}}{\hbar\omega}}$$

where $\hat{H}$ is Hamiltonian operator and using above equation (79) and (81), we get

$$\boxed{\hat{H} = \frac{\hbar\omega}{2}\left(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right)}$$

Now we will find some commutator

$$\left[\hat{a}, \hat{H}\right] = ??$$

$$\begin{aligned}
\left[\hat{a}, \hat{H}\right] &= \left[\hat{a}, \frac{\hbar\omega}{2}\left(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right)\right] \\
&= \frac{\hbar\omega}{2}\left[\hat{a}, \hat{a}\hat{a}^\dagger\right] + \frac{\hbar\omega}{2}\left[\hat{a}, \hat{a}^\dagger\hat{a}\right] \\
&= \frac{\hbar\omega}{2}\left(\left[\hat{a}, \hat{a}\right]\hat{a}^\dagger + \hat{a}\left[\hat{a}, \hat{a}^\dagger\right]\right) + \frac{\hbar\omega}{2}\left(\left[\hat{a}, \hat{a}^\dagger\right]\hat{a} + \hat{a}^\dagger\left[\hat{a}, \hat{a}\right]\right) \\
&= \frac{\hbar\omega}{2}\hat{a} + \frac{\hbar\omega}{2}\hat{a} \\
&= \hbar\omega\hat{a}
\end{aligned}$$

and another thing is

$$\left[\hat{a}^\dagger, \hat{H}\right] = ??$$

$$\begin{aligned}
\left[\hat{a}^\dagger, \hat{H}\right] &= \left[\hat{a}^\dagger, \frac{\hbar\omega}{2}\left(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right)\right] \\
&= \frac{\hbar\omega}{2}\left[\hat{a}^\dagger, \hat{a}\hat{a}^\dagger\right] + \frac{\hbar\omega}{2}\left[\hat{a}^\dagger, \hat{a}^\dagger\hat{a}\right] \\
&= \frac{\hbar\omega}{2}\left(\left[\hat{a}^\dagger, \hat{a}\right]\hat{a}^\dagger + \hat{a}\left[\hat{a}^\dagger, \hat{a}^\dagger\right]\right) + \frac{\hbar\omega}{2}\left(\hat{a}^\dagger, \hat{a}^\dagger]\hat{a} + \hat{a}^\dagger\left[\hat{a}^\dagger, \hat{a}\right]\right) \\
&= \frac{\hbar\omega}{2}(-1)\,\hat{a}^\dagger + \frac{\hbar\omega}{2}(-1)\,\hat{a}^\dagger \\
&= -\hbar\omega\hat{a}^\dagger
\end{aligned}$$

the value of commutator is

$$\boxed{\left[\hat{a}, \hat{H}\right] = \hbar\omega\hat{a}}$$

$$\boxed{\left[\hat{a}^\dagger, \hat{H}\right] = -\hbar\omega\hat{a}^\dagger}$$

Now we are going to start the calculation of energy eigenvalue.To obtain the energy levels of oscillator we have to calculate the matrix of Hamiltonian and then diagonalize it.The matrix of H would thus be a diagonal matrix.

$$\langle m|H|n\rangle = E_n\langle m|n\rangle = E_n\delta_{mn}$$

where $\langle m|$ and $|n\rangle$ are states or eigenvectors and E_n is energy eigenvalue of n^{th} state. Next,we shall evaluate the matrix of the product $\hat{a}^\dagger\hat{a}$

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle n\left|\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right|n\rangle = \frac{E_n}{\hbar\omega} - \frac{1}{2} \tag{12.6}$$

The matrix of $\hat{a}^\dagger\hat{a}$ can also be written as

$$\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \left|\hat{a}|n\rangle\right|^2 \geq 0 \tag{12.7}$$

from equation (82) and equation (83) we can write

$$\frac{E_n}{\hbar\omega} - \frac{1}{2} \geq 0$$

$$E_n \geq \frac{1}{2}\hbar\omega$$

for ground state of harmonic oscilator energy will be minimum (i.e. minimum energy of oscillator for $n = 0$)

$$E_{min} = E_0 = \frac{1}{2}\hbar\omega \tag{12.8}$$

Now consider the eigenvalue equation $H|n\rangle = E_n|n\rangle$.Operating from left by a,we get,$aH|n\rangle = E_n a|n\rangle$.But using above commutator relation we can write

$$\left[\hat{a}, \hat{H}\right]\left|n\right\rangle = \hbar\omega\hat{a}\left|n\right\rangle$$
$$\hat{a}\hat{H}\left|n\right\rangle - \hat{H}\hat{a}\left|n\right\rangle = \hbar\omega\hat{a}\left|n\right\rangle$$

$$\boxed{\hat{H}\left[a|n\rangle\right] = (E_n - \hbar\omega)\left[a|n\rangle\right]}$$

and similarly

$$\boxed{\hat{H}\left[a^\dagger|n\rangle\right] = (E_n + \hbar\omega)\left[a^\dagger|n\rangle\right]}$$

by using of above relation,if we take an eigenket $\hat{a}^\dagger|0\rangle$ of H then

$$\hat{H}\left[a^\dagger|0\rangle\right] = (E_0 + \hbar\omega)\left[a^\dagger|0\rangle\right]$$

that is,$\hat{a}^\dagger\left|0\right\rangle$ is eigenket of H with eigenvalue $E_0 + \hbar\omega = \frac{3}{2}\hbar\omega$. Repeated operation by $\hat{a}^\dagger$ raises the eigenvalue every time by $\hbar\omega$ consequently. In general we can write for $\hat{a}^\dagger\left|n\right\rangle$ eigenket of H corresponding to eigenvalue

$$E_n = E_0 + n\hbar\omega$$

$$\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega}$$

Where $n = 0, 1, 2, 3, ...$

$$Eigenket : \left|0\right\rangle, \hat{a}^\dagger\left|0\right\rangle, \left(\hat{a}^\dagger\right)^2\left|0\right\rangle, ...\left(\hat{a}^\dagger\right)^n\left|0\right\rangle$$

$$Eigenvalue : \frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, ...\left(n + \frac{1}{2}\right)\hbar\omega$$

12.2 calculations of expectations values using operator formalism

we know that

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \hat{p}\frac{i}{\sqrt{2m\omega\hbar}} \tag{12.9}$$
$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \hat{p}\frac{i}{\sqrt{2m\omega\hbar}} \tag{12.10}$$

adding two above equations and simplifying we get

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \tag{12.11}$$

subtracting above two equations and simplifying we get

$$\hat{p} = \frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}(\hat{a} - \hat{a}^\dagger) \tag{12.12}$$

where $\hat{a}$ is lowering operator and $\hat{a}^\dagger$ is raising operator

Eigenstates of a harmonic oscillator are orthogonal so $\langle n|m\rangle = 0$ for $n \neq m$ and 1 for $n = m$

On operating $\hat{a}$ on a given state n it gives

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \tag{12.13}$$

On operating $\hat{a}^\dagger$ on a given state n it gives

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{12.14}$$

Now calculating the expectation value of position operator $\hat{x}$

$$\begin{aligned}\langle\hat{x}\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle n|(\hat{a} + \hat{a}^\dagger)|n\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}}[\langle n|\hat{a}|n\rangle + \langle n|\hat{a}^\dagger|n\rangle] \\ &= \sqrt{\frac{\hbar}{2m\omega}}[\sqrt{n}\langle n|n-1\rangle + \sqrt{n+1}\langle n|n+1\rangle] \\ &= 0\end{aligned} \tag{12.15}$$

it is zero because of orthogonality condition

Now calculating the expectation value of momentum operator $\hat{p}$

$$\begin{aligned}\langle\hat{p}\rangle &= \frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}\langle n|(\hat{a} - \hat{a}^\dagger)|n\rangle \\ &= \frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}[\langle n|\hat{a}|n\rangle - \langle n|\hat{a}^\dagger|n\rangle] \\ &= \frac{1}{i}\sqrt{\frac{\hbar}{2m\omega}}[\sqrt{n}\langle n|n-1\rangle - \sqrt{n+1}\langle n|n+1\rangle] \\ &= 0\end{aligned} \tag{12.16}$$

it is also zero because of orthogonality condition

Now calculating the expectation value of $\langle \hat{x}^2 \rangle$

$$\begin{aligned}\langle \hat{x}^2 \rangle &= \frac{\hbar}{2m\omega}\langle n|(\hat{a}+\hat{a}^\dagger)(\hat{a}+\hat{a}^\dagger)|n\rangle \\ &= \frac{\hbar}{2m\omega}\langle n|(\hat{a}^2+\hat{a}^{\dagger^2}+\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a})|n\rangle\end{aligned} \tag{12.17}$$

now solving each component

$$\begin{aligned}\langle n|\hat{a}^2|n\rangle &= \sqrt{n}\langle n|\hat{a}|n-1\rangle \\ &= \sqrt{n}\sqrt{n-1}\langle n|n-2\rangle \\ &= 0\end{aligned} \tag{12.18}$$

$$\begin{aligned}\langle n|\hat{a}^{\dagger^2}|n\rangle &= \sqrt{n+1}\langle n|\hat{a^\dagger}|n+1\rangle \\ &= \sqrt{n+1}\sqrt{n+2}\langle n|n+2\rangle \\ &= 0\end{aligned} \tag{12.19}$$

$$\begin{aligned}\langle n|\hat{a}\hat{a^\dagger}|n\rangle &= \sqrt{n+1}\langle n|\hat{a}|n+1\rangle \\ &= \sqrt{n+1}\sqrt{n+1}\langle n|n\rangle \\ &= n+1\end{aligned} \tag{12.20}$$

$$\begin{aligned}\langle n|\hat{a^\dagger}\hat{a}|n\rangle &= \sqrt{n}\langle n|\hat{a}^\dagger|n-1\rangle \\ &= \sqrt{n}\sqrt{n}\langle n|n\rangle \\ &= n\end{aligned} \tag{12.21}$$

now it becomes

$$\begin{aligned}\langle \hat{x}^2 \rangle &= \frac{\hbar}{2m\omega}(n+1+n) \\ &= \frac{\hbar}{2m\omega}(2n+1) \\ &= \boxed{(n+\frac{1}{2})\frac{\hbar}{m\omega}}\end{aligned} \tag{12.22}$$

Now calculating expectation value of $\langle \hat{p}^2 \rangle$

$$\begin{aligned}\langle \hat{p}^2 \rangle &= \frac{-\hbar m\omega}{2}\langle n|(\hat{a}-\hat{a}^\dagger)(\hat{a}-\hat{a}^\dagger)|n\rangle \\ &= \frac{-\hbar m\omega}{2}\langle n|(\hat{a}^2+\hat{a}^{\dagger^2}-\hat{a}\hat{a}^\dagger-\hat{a}^\dagger\hat{a})|n\rangle\end{aligned} \tag{12.23}$$

from equation 12.18 ,12.19,12.20,12.21 it becomes

$$\begin{aligned}\langle \hat{p}^2 \rangle &= \frac{-\hbar m\omega}{2}(-(n+1)-n) \\ &= \frac{\hbar m\omega}{2}(2n+1) \\ &= \boxed{(n+\frac{1}{2})\hbar m\omega}\end{aligned} \tag{12.24}$$

let us now calculate uncertainity in position and momentum

Uncertaininty in position

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{\hbar}{m\omega}(n+\frac{1}{2})} \tag{12.25}$$

Uncertainity in momentum

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\hbar m\omega(n+\frac{1}{2})} \tag{12.26}$$

now **uncertainity product** becomes

$$\boxed{\Delta x\Delta p = (n+\frac{1}{2})\hbar} \tag{12.27}$$

12.3 Derivation of wave function using Algebraic method

Let ψ_0 be the value of the wave function representing the lowest state of the quantum harmonic oscillator.

$$\hat{a}\psi_0 = 0 \tag{12.28}$$

However $\hat{a}$ can be also written as follows,

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right) \tag{12.29}$$

Substituting eqn.12.29 into eqn.12.28 we get the following expression

$$\begin{aligned}\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0\\ \frac{d\psi_0}{dx} \quad = -\frac{m\omega}{\hbar}x\psi_0\end{aligned} \tag{12.30}$$

Integrating both the sides of the above obtained differential equation we get,

$$\begin{aligned}\int\frac{d\psi_0}{\psi_0} &= -\frac{m\omega}{\hbar}\int x\,dx\\ ln\psi_0 &= -\frac{m\omega}{2\hbar}x^2 + constant\\ \psi_0 &= Ae^{-\frac{m\omega}{2\hbar}x^2}\end{aligned} \tag{12.31}$$

On normalizing the above equation we obtain the value of constants,

$$\begin{aligned}1 &= |A|^2\int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}}\,dx\\ 1 &= |A|^2\sqrt{\frac{\pi\hbar}{m\omega}}\\ A &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\end{aligned} \tag{12.32}$$

Thus the value of wave function of the lowest state of the quantum harmonic oscillator can be given by-

$$\boxed{\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}} \tag{12.33}$$

Comparing it with the results obtained till now

$$\begin{aligned}
\hat{H}\psi_0 &= E_0\psi_0 \\
E_0\psi_0 &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}(\psi_0) + \frac{1}{2}m\omega^2 x^2\psi_0 \\
&= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}\right) + \frac{1}{2}m\omega^2 x^2\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} \\
E_0 &= \left(n + \tfrac{1}{2}\right)\hbar\omega
\end{aligned} \tag{12.34}$$

The result obtained by using Hamiltonian operator on the ground state wave function given by eqn.12.33 is the same as one obtained using operator method using actually solving the equation and the result is given by eqn.12.8. This shows that our result is in accordance with the previous developments done up to this point. In general the wave function for n^{th} state of harmonic oscillator can be obtained by using the raising operator on the ground state wave function ψ_0

$$\psi_n(x) = A_n(a^\dagger)^n\psi_0(x) \tag{12.35}$$

On normalising the above equation and using the results obtained in eq.12.13 and eq.12.14 we get the following expression,

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{n!}}(a^\dagger)^n\psi_0(x)} \tag{12.36}$$

Chapter 13

Quantum Hall Effect

13.1 Classical Hall Effect

13.1.1 Classical motion in B

$$m\frac{d\vec{v}}{dt} = -e\vec{v} \times \vec{B} \qquad \vec{v} = (\dot{x}, \dot{y}, 0), \vec{B} = (0, 0, \dot{z}) \tag{13.1}$$

$$m\ddot{x} = -eB\dot{y} \tag{13.2}$$

$$m\ddot{y} = eB\dot{x} \tag{13.3}$$

$$x(t) = X - R\sin(\omega_B t + \phi) \tag{13.4}$$

$$y(t) = Y + R\cos(\omega_B t + \phi) \tag{13.5}$$

$$\tag{13.6}$$

where, $\boxed{\omega_B = \frac{eB}{m}}$ is the cyclotron frequency.

13.1.2 Drude Model

$$\vec{J} = -en\vec{v} \tag{13.7}$$

where v is velocity of electrons crossing area A in time dt is $nvAdt$; each has charge $-e$ then current density is then $\vec{J}$.

Now,

$$\vec{v} = \frac{\vec{P}}{m} \tag{13.8}$$

$$= \frac{e\vec{E}\tau}{m} \tag{13.9}$$

$\because$ Using equations 13.7 and 13.9, Ohm's Law :

$$\vec{J} = \sigma\vec{E}$$

$$\therefore \boxed{\sigma = -\frac{e^2 n\tau}{m}}$$

In presence of B:

$$\text{Motion } m\frac{d\vec{v}}{dt} = e\vec{E} - e\vec{v}\times\vec{B}$$

$$\implies \frac{m\vec{v}}{\tau} + e\vec{v}\times\vec{B} = -e\vec{E}$$

$$\implies \vec{v} + \frac{e\tau}{m}\vec{v}\times\vec{B} = -\frac{e\tau}{m}\vec{E}$$

$\vec{v} = \frac{\vec{J}}{-en} \Rightarrow \dot{x} = \frac{J_x}{-en}, \dot{y} = \frac{J_y}{-en}$ and $\vec{v}\times\vec{B} = \hat{\imath}(-B\dot{y}) + \hat{\jmath}(B\dot{x})$

$$\implies \left(\dot{x} - \frac{e\tau}{m}B\dot{y}\right)\hat{\imath} + \left(\dot{y} + \frac{e\tau}{m}B\dot{x}\right)\hat{\jmath} = \left(\frac{e^2 n\tau}{m}\right)\vec{E}$$

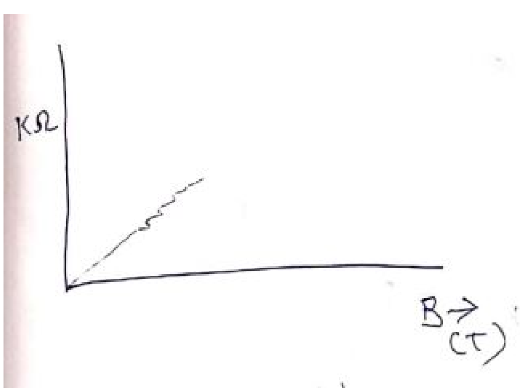
$$\Rightarrow \left(J_x - \left(\frac{eB}{m}\tau J_y\right)\right)\hat{\imath} + \left(J_y - \left(\frac{eB}{m}\tau J_x\right)\right)\hat{\jmath} = \left(\frac{e^2 n\tau}{m}\right)\vec{E}$$

$$\Rightarrow \begin{pmatrix} 1 & \omega_B\tau \\ -\omega_B\tau & 1 \end{pmatrix}\begin{pmatrix} J_x \\ J_y \end{pmatrix} = \sigma_D \begin{pmatrix} E_x \\ E_y \end{pmatrix}$$

$$\Rightarrow \rho = \frac{1}{\sigma_D}\begin{pmatrix} 1 & \omega_B\tau \\ -\omega_B\tau & 1 \end{pmatrix}$$

$$\vec{J} = \sigma\vec{E} \Rightarrow \boxed{\sigma = \frac{\sigma_D}{1+{\omega_B}^2\tau^2}\begin{pmatrix} 1 & -\omega_B\tau \\ \omega_B\tau & 1 \end{pmatrix}}$$

13.2 Quantum Hall Effect



$$F = evB\,;\, evB.L = E \to BL^2 = \frac{E.S}{e} = flux\,;\, E = \frac{V}{x}\,,\, B = EC = \frac{V}{t}$$

$$\frac{B}{\rho} = \frac{Field}{Density\,of\;Particle} = \frac{Field\;Density}{Particle} \approx \frac{\Phi_o}{v}$$

$$where\;\Phi_o = \frac{2\pi\hbar}{e} = \frac{h}{e} = flux\;quantum\;;v \to integer\;number$$

$$Resistivity\;\rho_{xy} = (\;\frac{h}{e})\;\frac{1}{e}\frac{1}{v}$$

13.2.1 Theory

In the presence of B,

$$H = \frac{1}{2m}(\;\vec{p} + e\vec{A})\;^2 = \frac{1}{2m}(\;m\vec{x})\;^2$$

where $\vec{p}$ is canonical momentum, e is field momentum and $m\vec{x}$ is mechanical momentum. In Heisenberg plane:

Mechanical momentum $m\vec{x} = \vec{\eta} = \vec{p} + e\vec{A}$ where,

$$\vec{p} \to [p_i, p_j] = 0 = [x_i, x_j] \quad \text{and} \quad [x_i, p_j] = i\hbar\delta_{ij}$$

$$\vec{\eta} = [\vec{\eta}_i, \vec{\eta}_j] = -ie\hbar\epsilon_{ijk}B_k \;\Rightarrow [\vec{\eta}_x, \vec{\eta}_y] = -ie\hbar B$$

$$\Rightarrow a = \frac{1}{\sqrt{2e\hbar B}}(\;\vec{\eta}_x - i\vec{\eta}_y)\;\;;a^+ = \frac{1}{\sqrt{2e\hbar B}}(\;\vec{\eta}_x + i\vec{\eta}_y)\;\Rightarrow [a, a^+] = 1$$

$$\Rightarrow H = \frac{1}{2m}\vec{\eta}.\vec{\eta} = \hbar w_B(\;a^+a + \frac{1}{2})\;\;where\;w_B = \frac{eB}{m}$$

Landau levels:

$$\Rightarrow E_\eta = \hbar w_B(\;\eta + \frac{1}{2})\;\;where\;\eta \to L$$

13.3 Schr$\ddot{o}$dinger's picture

$$\vec{\nabla} \times \vec{A} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} = B\hat{k} \quad \text{(where B is constant)}$$

$$\Rightarrow \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{k} = B\hat{k}$$

$$\Rightarrow \left[\frac{\partial\,(xB)}{\partial x} + 0\right]\hat{k} = B\hat{k}$$

$$\Rightarrow A_y = xB$$

$$\Rightarrow \vec{A} = xB\hat{j}$$

So, Hamiltonian $H = \frac{1}{2m}\left(\vec{p} + e\vec{A}\right)^2$

$$H = \frac{1}{2m}\left(p_x\hat{i} + (p_y + eBx)\,\hat{j}\right)^2$$

$$H = \frac{1}{2m}\left[p_x^2 + (p_y + eBx)^2\right]$$

$$guess \rightarrow \psi_k\,(x, y) = e^{iky} f_k\,(x)$$

System remains invariant under translation in y-direction. Similarly, stationary state $e^{iE\frac{t}{\hbar}}$ because $|\psi(t)|^2$ is constant.

$\Rightarrow$ The system remains invariant under time translation.

$$\hat{H}\Psi_k(x, y) = \frac{1}{2m}[p_x^2 + p_y^2 + 2p_y(eBx) + (eBx)^2]\Psi_k(x, y)$$

$$= \frac{1}{2m}[p_x^2 + (-i\hbar\frac{\partial^2}{\partial y^2}) + 2(eBx)(-i\hbar\frac{\partial}{\partial y}) + (eBx)^2]e^{iky}\Psi_k(x)$$

$$= \frac{1}{2m}[p_x^2 + \hbar^2k^2 + 2eBx\hbar k + (eBx)^2]\Psi_k(x, y)$$

$$\hat{H}\psi(x, y) = \frac{1}{2m}\left[p_x^2 + (\hbar k + eBx)^2\right]\psi_k(x, y) \tag{13.10}$$

$$= \frac{p_x^2}{2m} + \frac{e^2B^2}{2m}\left[x + k\left(\frac{\hbar}{eB}\right)\right]^2 \tag{13.11}$$

$$= \frac{p_x^2}{2m} + \frac{m}{2}\left(\frac{eB}{m}\right)^2\left[x + kl_B^2\right]^2 \tag{13.12}$$

Where,

$$\left(\frac{eB}{m}\right)^2 = \omega_B$$

$$\left[x + kl_B^2\right] = x'$$

$$\text{Magnetic Length } l_B = \sqrt{\frac{\hbar}{eB}}$$

$$\hat{H}\psi(x, y) = \frac{p_{x'}}{2m} + \frac{1}{2}kx'^2 \qquad k = m\omega_B \tag{13.13}$$

13.3.1 Repeat Harmonic oscillator problem

$$E_n = \hbar\omega_B\left(n + \frac{1}{2}\right)$$

$$\psi_{n,k}(x', y) \sim e^{iky} H_n(x') e^{-x'^2/2l_B^2}$$

13.4 Integer Quantum Hall Effect

$$\rho_{xy} = \left(\frac{h}{e}\right)\frac{1}{e}\left(\frac{1}{\nu}\right) \qquad \nu = 1, 2, 3\cdots \tag{13.14}$$

Comparing CHE and QHE, n needed for ν^{th} plateau,

$$\frac{h}{e^2}\frac{1}{\nu} = \frac{B}{ne} \tag{13.15}$$

$$\Longrightarrow \boxed{n = \frac{B}{\phi_0}\nu} \tag{13.16}$$

$$\phi_0 = \frac{h}{e} \text{ (flux quanta)} \tag{13.17}$$

Now in CHE,

$$\rho = \frac{1}{\sigma_D}\begin{pmatrix} 1 & \omega_B\tau \\ -\omega_B\tau & 1 \end{pmatrix} \tag{13.18}$$

$$\rho_{xx} = \rho_{yy} = 1/\sigma_D \tag{13.19}$$

$$\rho_{xy} = -\rho_{yx} = \frac{\omega_B\tau}{\sigma_D} \tag{13.20}$$

$$\sigma = \frac{\sigma_D}{1+\omega_B^2\tau^2}\begin{pmatrix} 1 & -\omega_B\tau \\ \omega_B\tau & 1 \end{pmatrix} \tag{13.21}$$

$$\sigma_{xx} = \sigma_{yy} = \frac{\sigma_D}{1+\omega_B^2\tau^2} \tag{13.22}$$

$$\sigma_{xx} = \frac{\rho_{xx}}{\rho_{xx}^2+\rho_{yy}^2} \tag{13.23}$$

$$\sigma_{xy} = -\frac{\rho_{xy}}{\rho_{xx}^2+\rho_{xy}^2} \tag{13.24}$$

$$QHE \Longrightarrow \rho_{xy} = \frac{\phi_0}{e}\frac{1}{2} \to \text{plateau}$$

$$\rho_{xx} = 0 \text{ with spike}$$

If $\rho_{xy} = 0$, then traditional conductivity and resistivity relation,

$$\boxed{\sigma_{xx} = \frac{1}{\rho_{xx}}} \tag{13.25}$$

But in the presence of B, if $\rho_{xx} = 0$, then $\boxed{\sigma_{xx} = 0}$!

$$\rho_{xx} = 0 \implies \tau \to \alpha \text{ or no dissipation (perfect conductor)}$$

$$\sigma_{xx} = 0 \implies \text{ no electrons move (insulator)}$$

$$\text{And } \rho_{xx} = 0 \implies \boxed{\sigma_{xy} = -\frac{1}{\rho_{xy}}} \tag{13.26}$$

13.5 Conductivity in QM (a baby version)

In presence of magnetic field electron momentum $\left(m\dot{x} = \vec{p} + e\vec{A}\right)$ has two parts- mechanical momentum ($\vec{p}$) and field momentum $\left(e\vec{A}\right)$.

$$m\dot{x} = \vec{p} + e\vec{A} \tag{13.27}$$

$$\text{Current} = I = e\dot{x} \tag{13.28}$$
$$= \frac{e}{m}\sum\langle\psi| - i\hbar\vec{\nabla} + e\vec{A}|\psi\rangle \tag{13.29}$$

$$\text{Now } I_x = -\frac{e}{m}\sum_{n=1}^{v}\sum_{k}\langle\psi_{n,k}| - i\hbar\frac{\delta}{\delta x}|\psi_{n,k}\rangle = 0 \tag{13.30}$$

momentum expectation of harmonic oscillation vanish.

$$I_y = \frac{-e}{m}\sum_{n=1}^{v}\sum_{k}\langle\psi_{n,k}| - i\hbar\frac{\delta}{\delta y} + exB|\psi_{n,k}\rangle \tag{13.31}$$

$$= \frac{-e}{m}\sum_{n=1}^{v}\sum_{k}\langle\psi_{n,k}|\hbar K + exB|\psi_{n,k}\rangle \tag{13.32}$$

$$\text{Now } \langle\psi_{n,k}|x|\psi_{n,k}\rangle = \frac{-\hbar K}{eB} + \frac{-mE}{eB^2} \quad \text{because x is shifting coordinate} \tag{13.33}$$

$$I_y = \frac{-e}{m}\sum_{n=1}^{v}\sum_{k}\langle|\frac{mE}{eB^2}xeB|\rangle \tag{13.34}$$

$$= -ev \sum_k \left(\frac{E}{B}\right) \tag{13.35}$$

$$\frac{I_y}{A} = J_y = \left(-\frac{e}{\phi_0} v\right) E_x \qquad \text{as } \sum_k = N = \frac{AB}{\phi_0} \tag{13.36}$$

$$\boxed{\sigma_{xy} = \frac{ev}{\phi_0}} \tag{13.37}$$

$$\boxed{\rho_{xy} = \frac{1}{\sigma_{xy}} = \left(\frac{\phi_0}{e}\frac{1}{v}\right)} \tag{13.38}$$

Explained

Chapter 14

Hydrogen Atom

S.E.

$$\nabla^2\psi(r) + \frac{2m}{\hbar^2}(E-V)\psi(r) = 0$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \qquad (14.1)$$

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

$$\frac{r^2 sin^2\theta}{R\Theta\Phi} \implies \frac{sin^2\theta}{R}\frac{d}{dr}\left(\frac{r^2 dR}{dr}\right) + \frac{sin\Theta}{\Theta}\frac{d}{d\theta}\left(sin\theta\frac{d\Theta}{d\theta}\right) + \frac{2m}{\hbar^2}\left[E - V(r)\right]r^2 sin\theta = -\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}$$

Assuming $\frac{d^2\Phi}{d\phi^2} = -m^2\Phi(\phi) \implies \Phi(\phi) = Ae^{\pm im\phi} = \frac{1}{\sqrt{2\pi}}e^{im\phi}$

m $= 0, \pm1, \pm2, \pm3...$ as $\Phi(\phi) = \Phi(\phi + 2\pi) \implies e^{\pm im2\pi} = 1$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2m}{\hbar^2}(E-V)r^2 = -\frac{1}{\Theta sin\theta}\frac{d}{d\theta}\left(sin\theta\frac{d\Theta}{d\theta}\right) + \frac{m^2}{sin^2\theta} = \lambda = l(1+l)$$

$$\implies \frac{1}{sin\theta}\frac{d}{d\theta}\left(sin\theta\frac{d\Theta}{d\theta}\right) + \left(\lambda - \frac{m^2}{\sin^2\theta}\right)\Theta = 0$$

$$\implies (H)(\theta) = N_{lm}P_l^{|m|}(\cos\theta).$$

physical acceptable solution

$$\lambda = l(l+1), \quad where \quad l = 0, \pm1, \pm2, \pm3\cdots\cdots$$

$$m = 0, \pm1, \pm2, \cdots \pm \mathrm{l}(m_{max})$$

Radial Part:-

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}\left[E-\frac{l(l+1)\hbar^2}{2\mu r^2}+\frac{kze^2}{r}\right]R$$

$$n = l + n' + 1 = \lambda(terminator \quad condition)$$

$$where \quad \lambda = \frac{kze^2}{\hbar}\sqrt{\frac{\mu}{-2E}}$$

$$\Rightarrow E_n = -\left(\frac{\mu z^2 e^4}{k^2 2\hbar^2}\right)\frac{1}{n^2} \quad \text{with } k = 4\pi\epsilon_0$$

principal quantum no. $n = 1, 2, 3, \cdots\cdots$

where highest possible of l is $l_{\max} = n - 1$

Radial wave function

$$R_{nl}(\gamma) = -\left\{\left(\frac{2Z}{na_n}\right)^3\frac{(n-l-1)!}{2n[(n+1)!]^3}\right\}^{1/2} e^{-\rho/2}\rho^L L_{n+l}^{2l+1}(\rho)$$

with

$$\rho = \sqrt{\frac{-8\mu E}{\hbar^2}}r$$

$$a_H = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2} = \text{ Bohr radium}$$

So total wave function

$$\psi_{n,l,m}(\gamma,\theta,\phi) = R_{n,L}(\gamma)\times(\Theta)_{l,m}(\theta)\times e^{\mathrm{im}\phi}$$

where $n = 1, 2, 3, \cdots\cdots$
for fixed $n, l = 0, 1, 2, \cdots, (n-1)$
for fixed $l, m = 0, \pm1, \pm2, \cdots, \pm l$

Chapter 15

Scattering Theory

15.1 Page1-4

$\sigma(\theta,\phi) = \frac{\eta d\Omega}{N}$;   n is no. of scattered particle into solid angle $d\Omega$

N is incident particle no.

Solid angle dΩ = $\frac{r \sin\theta r d\theta d\phi}{r^2} = \sin\theta \, d\theta \, d\phi$

Differential scattering cross section:

$\sigma(\theta, \phi) \approx \frac{d\sigma}{d\Omega}$

Total cross section:

$\sigma(\theta, \phi)_{total} = \int \frac{d\sigma}{d\Omega} d\Omega$

$\sigma(\theta, \phi)_{total} = \int\limits_0^{\pi} \sin\theta \, d\theta \int\limits_0^{2\pi} \frac{d\sigma(\theta,\phi)}{d\Omega} \, d\phi$

if ϕ = Symmetric case,

$\frac{d\sigma(\theta,\phi)}{d\Omega} = \frac{d\sigma(\theta)}{d\Omega}$

The total cross-section is given by:

$$\sigma_{total} = 2\pi \int_0^{\pi} \sigma(\theta) \sin\theta d\theta$$

schodengers equation:

$\frac{\hbar^2}{2M}\bar{\Delta}^2\psi + v(r)\psi = E\psi$

$\mu = \frac{mM}{m+M}$

In initial stage $\rightarrow$ incident wave $\psi_i \approx e^{iKZ}$(where $v(r) \rightarrow 0$) (Plane wave)

In final stage $\rightarrow$ spherical wave $\rightarrow e^{i\bar{k}.\bar{r}}$with scattering amplitude $f(\theta, \phi)$

so

$$\psi_i \to Ae^{ikz}$$

$$\psi_f \to Af(\theta)\frac{e^{ikr}}{r}$$

$$J_i = \frac{\hbar k|A|^2}{\mu}$$

$\nearrow$

Current density

$\searrow$

$$J_s = \left(\frac{\hbar k}{\mu}\right)\left|\frac{Af(\theta)}{r}\right|^2$$

$$\frac{d\sigma}{d\Omega} = \frac{Js(\text{number of scattered particles/area/time})}{Ji(\text{number of incident particles/area/time})} \times r^2(\text{area /unit solid angle})$$

$$r^2 = \frac{(rsin\theta d\phi)(rd\phi)}{d\Omega}$$

$$= |f(\theta)|^2$$

$$e^{ikz} = \sum_{l=0}^{\alpha} i^l(2l+1)J_l(kr)P_l(cos\theta)$$

$$J_l(x) = \text{Spherical Bessel Function}$$

$$P_l(x) = \text{Legendre Polynomial}$$

Bauer's Formula

$$\text{Asymptotically, } J_l(kr) \xrightarrow[r\to\alpha]{} \frac{1}{kr}sin(kr - \frac{l\pi}{2})$$

$$e^{ikz} = \sum_{l=0}^{\alpha} \frac{i^l(2l+1)}{2ik}P_l(cos\theta)\frac{1}{r}[e^{ikr-il\frac{\pi}{2}}]$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi$$

Let us consider $\psi(r,\theta) = R_l(r)P_l(\cos\theta)$.

So, the radial equation is given by:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}R_l\right) + \left(\frac{2\mu E}{\hbar^2} - \frac{2\mu V}{\hbar^2} - \frac{l(l+1)}{r^2}\right)R_l = 0$$

Outside the range of V, i.e., $V \to 0$, the equation becomes:

$$\frac{d^2}{dr^2}R_l + \frac{2}{r}\frac{d}{dr}R_l + \left[k^2 - \frac{l(l+1)}{r^2}\right]R_l = 0, \textbf{ where } k^2 = \frac{2\mu E}{\hbar^2}\textbf{.}$$

$\eta_l(kr)$ - Spherical Neumann's function
$J_l(kr)$ - Spherical Bessel's function

$$R_l(kr) \xrightarrow{r\to\alpha} \frac{A'}{kr}\sin(kr - \frac{\pi}{2}) + \frac{B'}{kr}\cos(kr - \frac{l\pi}{2}) = \frac{A_l}{kr}\sin(kr - \frac{l\pi}{2} + S_l)$$

$$\Psi(r,\theta) = \sum_{l=0}^{\alpha}\frac{A_l}{kr}\sin\left(kr - \frac{l\pi}{2} + S_l\right)P_l(\cos\theta)$$

$$e^{ikz} + \frac{f(\theta)e^{ikz}}{r} = \sum_{l=0}^{\alpha}(2l+1)\frac{e^{ikr}}{kr}i^l\sin\left(kr - \frac{l\pi}{2}\right)P_l(\cos\theta) + \frac{f(\theta)e^{ikr}}{r}$$

$$\sin\left(kr - \frac{l\pi}{2}\right) = \frac{e^{i(kr-\frac{l\pi}{2})} - e^{-i(kr-\frac{l\pi}{2})}}{2i}$$

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$$A_l = i^l(2l+1)e^{iS_l}$$

$$\sum_{l=0}^{\infty}\frac{(2l+1)i^l e^{-\frac{iln}{2}}}{2ikr}P_l(\cos\theta)+\frac{f(\theta)}{r}=\sum_{l=0}^{\infty}\frac{(2l+1)i^l e^{-\frac{iln}{2}}e^{2i\delta_l}}{2ikr}P_l(\cos\theta)$$

$$f(\theta)=\sum_{l=0}^{\infty}\frac{(2l+1)i^l e^{-\frac{iln}{2}}(e^{2i\delta_l}-1)}{2ik}P_l(\cos\theta)$$

$$\because i^l=e^{\frac{i\pi l}{2}}\quad and\quad e^{2i\delta_l}-1=e^{i\delta l}(e^{i\delta_l}-e^{-i\delta_l})=2ie^{i\delta_l}\sin\delta_l$$

$$f(\theta)=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}P_l(\cos\theta)\sin\delta_l$$

$$\psi(r,\theta)=\sum_{l=0}^{\infty}\frac{A_l}{kr}\sin(Kr-\frac{l\pi}{2}+\delta_l)P_l(\cos\theta)$$

$$=\sum_{l=0}^{\infty}\frac{i^l(2l+1)}{2iKr}[e^{i(Kr-\frac{l\pi}{2}+2\delta_l)}]$$

15.2 Pages 5-6

Quantum scattering, a phenomena inherent in particle behaviour, is crucial in understanding fundamental interactions at the quantum level. When particles collide with a potential, their trajectories change, resulting in complicated dispersion patterns. Quantum scattering analysis comprises a combination of mathematical terms, physical principles, and experimental findings.

The use of partial waves is an important idea in the study of quantum scattering since it allows for the decomposition of the total scattering amplitude into simpler components with various angular momentum values.

From the above calculations:

$$\frac{d\sigma}{d\Omega}=|f(\theta)|^2, f(\theta)=\sum_{i=1}^{\infty}(2l+1)f_l(k)P_l(cos\theta) \tag{15.1}$$

From the expression for $\frac{d\sigma}{d\Omega}$, we obtain the total scattering cross-section:

$$\sigma_{tot}=\int d\sigma=\int|f(\theta)|^2\,d\Omega \tag{15.2}$$

With orthogonality relation $\int d\Omega P_l(cos\theta)P_{l'}(cos\theta)=\frac{4\pi}{2l+1}\delta_{ll'}$,

$$\sigma_{tot}=\sum_{l,l'}(2l+1)(2l'+1)f_l*(k)f_{l'}(k)\int d\Omega P_l(cos\theta)P_{l'}(cos\theta) \tag{15.3}$$

$$\sigma_tot = 4\pi \sum_l (2l+1)|f_l(k)|^2 \tag{15.4}$$

and,

$$f(\theta) = \sum_{i=1}^{\infty} (2l+1) f_l(k) P_l(cos\theta) \tag{15.5}$$

Making use of the relation $f_l(k) = \frac{1}{2ik}(e^{2i\delta_l(k)} - 1) = \frac{e^{i\delta_l(k)}}{k} sin\delta_l$,

$$\sigma_tot = \frac{4\pi}{k^2} \sum_{i=1}^{\infty} (2l+1) sin^2\delta_l(k) \tag{15.6}$$

Since $P_l = 1, f(0) = \Sigma_l (2l+1) f_l(k) = \Sigma_l (2l+1) \frac{e^{i\delta_l(k)}}{k} sin\delta_l$,

$$Imf(0) = \frac{k}{4\pi}\sigma_{tot} \tag{15.7}$$

This is the optical theorem.

....

15.3 Attractive square well potential

The potential in an attractive square well is given

$$V(r) = \begin{cases} -V_0, & 0 < r < a \\ 0, & r > a. \end{cases}$$

We write down the radial part of schrödingers equation.

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{dr}) + \frac{2\mu}{\hbar^2}(E+V_0)R - \frac{l(l+1)}{r^2}R = 0. \tag{15.8}$$

Substituting $R = \frac{u}{r}$ in equation 15.8 we get

$$\frac{d^2u}{dr^2} + \left[\frac{2\mu E}{\hbar^2} + \frac{2\mu V_0}{\hbar^2} - \frac{l(l+1)}{r^2}\right]u = 0.$$

S-state (l=0)

$$\frac{d^2u}{dr^2} + k_1^2 u = 0 \text{ where } k_1 = \frac{2\mu}{\hbar^2}(E+V_0), r < a$$
$$\frac{d^2u}{dr^2} + k^2 u = 0 \text{ where } k = \frac{2\mu E}{\hbar^2}, r > a.$$

Solution:-

$$u = \begin{cases} A\sin(k_1 r), & r < a \\ C\sin(kr) + D\cos(kr) = B\sin(kr+\delta_0), & r > a. \end{cases}$$

$$R = \frac{u}{r} = \frac{\cos k_1 r}{r} \rightarrow \alpha eatr \rightarrow 0$$

Function should be continuous and differentiable at a. We therefore get the following conditions

$$A\sin(k_1 a) = Bsin(ka+\delta_0) \tag{15.9}$$

$$A\cos(k_1 a) = Bk\cos(ka+\delta_0). \tag{15.10}$$

Dividing the above 2 equations,

$$\begin{aligned} \tan(ka+\delta_0) &= \frac{k}{k_1}\tan(k_1 a) \\ \delta_0 &= \tan^{-1}\left[\frac{k}{k_1}\tan(k_1 a)\right] - ka \\ \therefore \sigma &= \frac{4\pi}{k^2}\sin^2(\delta_0). \end{aligned}$$

At low energy $[ka \longrightarrow 0 \Rightarrow \tan(ka) \longrightarrow ka]$:-

$$\begin{aligned} \tan(ka+\delta_0) &= \frac{k}{k_1}\tan(k_1 a) \\ \frac{\tan(ka)+\tan(\delta_o)}{1-\tan(ka)\tan(\delta_o)} &= \frac{k}{k_1}\tan(k_1 a) \\ \tan(ka)+\tan(\delta_o) &= \frac{k}{k_1}\tan(k_1 a) - \frac{k}{k_1}\tan(ka)\tan(\delta_o)\tan(k_1 a) \\ \left[1+\frac{k}{k_1}\tan(ka)\tan(k_1 a)\right]\tan(\delta_o) &= \frac{k}{k_1}\tan(k_1 a) - \tan(ka) \\ \tan(ka) &\Rightarrow ka \\ \lim ka \longrightarrow 0, \tan\delta_o &= ka\left[\frac{\tan(k_1 a)}{ka} - 1\right] \end{aligned}$$

$$\begin{aligned} \text{at } k_1 a = \frac{\pi}{2}, &\tan\delta_o \rightarrow \infty \Rightarrow \delta_o = \frac{\pi}{2} \\ \sigma = \frac{4\pi}{k^2}\sin^2\delta_o &\rightarrow \sigma_{max} = \frac{4\pi}{k^2} \longrightarrow \end{aligned}$$

This effect is called Resonance

Behavior of σ near resonance energy E_R :-

Let $E = E_R = \frac{\hbar^2 k_R^2}{2\mu}$, $\sin\delta_o(E=E_r) \rightarrow 1$, $\cos\delta_o(E=E_r) \rightarrow 0$

Using Taylor's series,

$$\begin{aligned}
\sin(\delta_o(E)) &= \sin(\delta(E = E_R)) + \left[\frac{\partial}{\partial E}\sin(\delta_o)\right]_{E=E_R}(E - E_R) \\
&= \sin(\delta(E_R)) + \cos(\delta_o(E = E_R))(\frac{\partial}{\partial E}\delta_o)_{E=E_R}(E - E_R) \\
&\because \sin(\delta(E_R)) \to 1, \cos\delta_o(E_R) \to 0 \\
&= 1 \\
\cos\delta_0 &= \cos\delta_0(E + E_R) + \left[\frac{\partial}{\partial E}\cos\delta_0(E)\right]_{E=E_R}(E - E_R) \\
&= \cos\delta_0(E_R) - \sin\delta_0(E_R)\left[\frac{\partial\delta_0(E)}{\partial E}\right]_{E=E_R}(E - E_R) \\
\cos\delta_0(E) &= -\frac{2}{\Gamma}(E - E_R)
\end{aligned}$$

Where $\left|\frac{d\delta_0}{dE}\right|_{E=ER} = \frac{2}{\Gamma}$

Scattering amplitude,

$$\boxed{f(\theta, E) = \frac{1}{k}e^{i\delta_0(E)\sin\delta_0(E)}}$$

$$\begin{aligned}
f(\theta, E) &= \frac{1}{K}\frac{\sin\delta_0(E)}{[\cos\delta_0(E) - i\sin\delta_0(E)]} \\
&= \frac{1}{K}\frac{1}{\left[-\frac{2}{\Gamma}(E - E_R)\right] - i} \\
&= -\frac{1}{K}\frac{\frac{\Gamma}{2}}{(E - E_R) + i\frac{\Gamma}{2}} \\
&\Rightarrow \boxed{\frac{d\sigma}{d\Omega} = |f(\theta, E)|^2 = \frac{1}{K^2}\frac{\frac{\Gamma^2}{4}}{(E - E_R)^2 + \frac{\Gamma^2}{4}}} \\
&\Rightarrow \sigma = \int\frac{d\sigma}{dr}d\Omega = \frac{4\pi}{k^2}\frac{\frac{\Gamma^2}{4}}{(E - E_R)^2 + \frac{\Gamma^2}{4}}
\end{aligned}$$

<u>Scattering Length</u>

$$a = \lim_{E\to 0}[-f(\theta)] = \lim_{E\to 0} -\frac{e^{(i\delta_0)}}{K}sin\delta_0$$

if V(r) is weak => $K_1 \to 0$ like $K \to 0$, so $tan\delta_0 = Ka[\frac{tanK_1a}{K_1a} - 1] = 0 \Rightarrow \delta_0 \to 0$

Now $\lim_{\delta_0\to 0} e^{i\delta_0}sin\delta_0 \to \delta_0 \Rightarrow \boxed{a = -\frac{\delta_0}{K}} \Rightarrow \delta_0 \Rightarrow -ka$

$\therefore \sigma_0 = \frac{4\pi}{K^2} sin^2 \delta_0$

$\therefore \lim_{E\to 0} \sigma_0 = \frac{4\pi}{K^2}(Ka)^2$

$= 4\pi a^2$

15.4 Hand Sphere Scattering

$$\begin{aligned} V(r) &= \infty \quad \text{for } 0 \le r \le a \longrightarrow \psi_1(r) \to 0 \\ &= 0 \quad \text{for } r > a \longrightarrow \psi_2(r) \to ? \end{aligned}$$

for $r > a$, $\frac{d^2u}{dr^2} + \frac{2\mu E}{\hbar^2} u = 0$

$k^2 = \frac{2\mu E}{\hbar^2}$

$\Rightarrow u = B\sin(kr + \delta_0)$

Continuity, $\left|\psi_2(r) = \frac{B}{r}\sin(kr + \delta_0)\right|_{r=a} = \psi_1(r = a)$

$\Rightarrow \frac{B}{a}\sin(ka + \delta_0) = 0$

$\Rightarrow \boxed{\delta_0 = n\pi - ka}$

$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta_0$

$\frac{4\pi}{k^2}\sin^2 ka \qquad \because \sin(n\pi - ka) = \sin(ka)$

$\boxed{\sigma_0 = 4\pi a^2}$ when $k \to 0$

Integral equation (Born approximation)

For potential $V(r)$,

S.E $(\nabla^2 + k^2)\,\psi(r) = V(r)\,\psi(r)$ where $V(r) = \frac{2\mu\, V(r)}{\hbar^2}$ and $k^2 = \frac{2\mu E}{\hbar^2}$

Using the plane incident wave and unknown scatter wave , we get

$(\nabla^2 + k^2)\,(e^{i\vec{k}\,\vec{r}} + \psi_S) = V(r)\,\psi(r)$

$(\nabla^2 + k^2)\,\psi_s = V(r)\,\psi(r) = -\rho(r)$ since $(\nabla^2 + k^2)\,e^{i\vec{k}\,\vec{r}} + \psi_S = 0$
In homogeneous equation

Using Green's function method ,

$(\nabla^2 + k^2)\,G(r, r') = S(r - r') \to G(r, r') = e^{\frac{i\vec{k}\cdot(\vec{r}-\vec{r'})}{4\pi|\vec{r}-\vec{r'}|}}$

$\psi_s = \int G(r, r')\rho(r')\,dr'$

$\psi_s = -\frac{i}{4\pi}\int e^{\frac{i\vec{k}\cdot(\vec{r}-\vec{r'})}{|\vec{r}-\vec{r'}|}}\,V(\vec{r'})\psi(\vec{r'})\,d\vec{r'}$

Now $|\vec{r}-\vec{r'}| \simeq r - r \cdot \vec{r'} + ...$
Therefore, $k|\vec{r}-\vec{r'}| = kr - k\hat{r}\cdot\vec{r'} = kr - \vec{k'}\cdot\vec{r'}$. where $\vec{k'} = k\hat{r}$ is the final wave vector
Now $\psi_s = -\frac{1}{4\pi}\int \frac{e^{i(kr-\vec{k'}\cdot\vec{r'})}}{r} V(\vec{r'})\psi(\vec{r'})\, d\vec{r'} = \frac{e^{ikr}}{r} f(\theta)$

$$\boxed{f(\theta) = -\frac{1}{4\pi}\int e^{i(-\vec{k'}\cdot\vec{r'})}\, V(r')\psi(r')\, dr'}$$

Example:
Coulomb Potential $V(r') = -\frac{\alpha}{r'}\, e^{-\alpha r'}$ $[Screening function]$

$$f(\theta) = \frac{2\mu}{\hbar^2}\int_0^\alpha \frac{\sin(qr')}{qr'}\frac{\alpha}{r'} e^{-\alpha r'} r'^2\, dr'$$
$$= \frac{2\mu\alpha}{\hbar^2}\frac{1}{q}\int_0^\alpha \sin(qr') e^{-\alpha r'}\, dr'$$
$$= \frac{2\mu\alpha}{\hbar^2 q}\frac{q}{q^2+\alpha^2}$$
$$= \frac{2\mu\alpha}{\hbar^2 q^2} \qquad when \quad \alpha \to 0 (\text{no screen}) \text{ or } q \gg \alpha$$

$\therefore \frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{4\mu^2\alpha^2}{\hbar^4 q^4}$ where $\alpha = ZZ'e^2$ $q = 2ksin(\frac{\theta}{2})$

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{\mu^2 Z^2 Z'^2 e^4}{4\hbar^4 k^4 (sin(\frac{\theta}{2}))^4}}$$ Rutherford's scattering formula

Born Approximation:

$\Psi(r) = e^{i\vec{k'}\cdot\vec{r'}} - \frac{e^{ik\cdot r}}{r} f(\theta)$ *where* $f(\theta) = -\frac{1}{4\pi}\int e^{-i\vec{k'}\cdot\vec{r'}}\, \upsilon(r')\psi(r')\, dr'$

1st Born approximation:

Assume, $\Psi(r') = e^{i\vec{k}\cdot\vec{r'}}$

$$f(\theta) = -\frac{1}{4\pi}\int e^{i(\vec{k}-\vec{k'})\cdot\vec{r'}}\, \upsilon(r') d\vec{r'}$$

Now, $\vec{q} = \vec{k} - \vec{k'}$

$\implies |\vec{q}| = 2\text{ksin}(\frac{\theta}{2})$ *and* $\vec{q}\cdot\vec{r'} = qr'cos(\theta')$

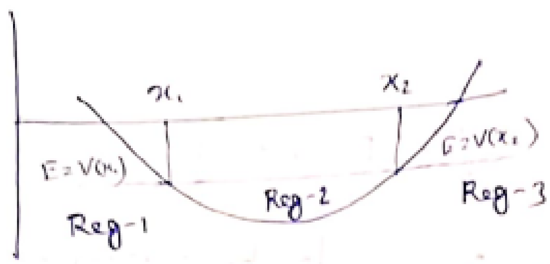
$$So, f(\theta) = -\frac{1}{4\pi}\int e^{iqr'cos(\theta')}\, \upsilon(r') d\vec{r'}$$
$$= -\frac{1}{4\pi}\int e^{iqr'cos(\theta')}\, \upsilon(r') r'^2 d\vec{r'} sin(\theta) d\theta d\Phi$$

$\upsilon(r') = \frac{2\mu}{\hbar^2} V(r')$

$\int d\phi = 2\pi \quad and \quad \int e^{iqr' cos(\theta)} sin\theta d\theta = \frac{2sin(qr')}{qr'}$

$$\boxed{f(\theta) = -\frac{2\mu}{\hbar^2}\int_0^\alpha \frac{\sin(qr')}{qr'} V(r') r'^2 \, dr'} \quad where \quad q = 2ksin(\tfrac{\theta}{2})$$

....


x_1
x_2
E = V(x₁)
E = V(x₂)
Reg-1
Reg-2
Reg-3

Chapter 16

Time Independent Perturbation Theory

16.1 page1-3

Unperturbed part $H^0\ \psi_n^0 = E_n^0\ \psi_n^0$, all 'n' are orthogonal to each other

Total Hamiltonian H = $H^0 + H'$ (small perturbation)

Let us assume H = $H^0 + \lambda H'$ where $\lambda \uparrow_0^1$

Consider the expansion → $E_n = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots$

$$\psi_n = \psi_n^0 + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \ldots$$

where $H\psi_n = E_n\psi_n$

$$\implies (H^0 + \lambda H')(\psi_n^0 + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \ldots) = (E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots)(\psi_n^0 + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \ldots)$$

$$\implies H^0\psi_n^0 = E_n^0\psi_n^0 \tag{16.1}$$

$$\implies \langle\psi_n^0|H^0\rangle = \langle\psi_n^0|E_n^0\rangle \tag{16.2}$$

$$\lambda\ coefficient \to H'\psi_n^0 + H^0\psi_n^{(1)} = E_n^{(1)}\psi_n^0 + E_n^0\psi_n^{(1)} \tag{16.3}$$

$$\lambda^2\ coefficient \to H'\psi_n^{(1)} + H^0\psi_n^{(2)} = E_n^{(2)}\psi_n^0 + E_n^{(1)}\psi_n^{(1)} + E_n^0\psi_n^{(2)} \tag{16.4}$$

By taking ket of equation 16.3 with $\langle\psi_n^0|$

First order correction $\langle\psi_n^0|(16.3) \implies \boxed{E_n^{(1)} = \langle\psi_n^0|H'|\psi_n^0\rangle}$, using (16.2)

1^{st} order energy

$$\text{Wave function} \quad \boxed{\psi_n^{(1)} = \sum_{l=1}^{\alpha} a_l \psi_l^0} \tag{16.5}$$

$$\Longrightarrow_{m\neq n} \langle \psi_m^0 | (16.3)$$

$$\Longrightarrow \langle \psi_m^0 | H' | \psi_n^0 \rangle + \sum_{l=1}^{\alpha} a_l E_l^0 \langle \psi_m^0 | \psi_l^0 \rangle = E_n^{(1)} \langle \psi_m^0 | \psi_n^0 \rangle + \sum_{l=1}^{\alpha} a_1 E_n^0 \langle \psi_m^0 | \psi_l^0 \rangle$$

$$\Longrightarrow \langle \psi_m^0 | H' | \psi_n^0 \rangle + a_m E_m^0 = a_m^0 E_n^0$$

$$\boxed{\Longrightarrow a_m = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)}} \qquad \text{Except } a_n \text{ all coefficients can be obtained.}$$

$$\psi_n^{(1)} = \sum_{l}^{1} \frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_l^0} | \psi_l^0 \rangle \qquad \text{prime} \implies l \neq n$$

So, $E_n = E_n^0 + E_n^{(1)} + E_n^{(2)}$

$$\boxed{E_n = E_n^0 + \langle \psi_n^0 | H' | \psi_n^0 \rangle + \sum_{l}^{l\neq n} \frac{|\langle \psi_n^0 | H' | \psi_l^0 \rangle|^2}{(E_n^0 - E_l^0)}} \tag{16.6}$$

$$\begin{aligned}
\psi_n &= \psi_n^0 + \psi_n^{(1)} + \psi_n^{(2)} \\
&= \psi_n^0 + \sum_{l}^{n\neq l} a_l \psi_l^0 + \sum_{l}^{l\neq n} b_l \psi_l^0 \\
&= \psi_n^0 + \sum_{l}^{n\neq l} \frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_l^0)} | \psi_l^0 \rangle + \sum_{l}^{l\neq n} \left[\sum_{k}^{k\neq n} \frac{\langle \psi_k^0 | H' | \psi_n^0 \rangle \langle \psi_l^0 | H' | \psi_k^0 \rangle}{(E_n^0 - E_k^0)(E_n^0 - E_l^0)} - \frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle \langle \psi_n^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_l^0)^2} \right] | \psi_l^0 \rangle
\end{aligned}$$

second-order correction
By doing ket of equation 16.4 with $\langle \psi_n^0 |$

$$\langle \psi_n^0 | (16.4) \implies \langle \psi_n^0 | H' | \psi_n^{(1)} \rangle + \langle \psi_n^0 | H^0 | \psi_n^{(2)} \rangle = E_n^{(2)} \langle \psi_n^0 | \psi_n^0 \rangle + E_n^{(1)} \langle \psi_n^0 | \psi_n^{(1)} \rangle + \langle \psi_n^0 | E_n^0 | \psi_n^{(2)} \rangle$$

(because of (16.2))

$$\text{Since} \quad \psi_n^{(1)} = \sum_{l=1}^{\infty} a_l | \psi_l^0 \rangle + a_n | \psi_n^0 \rangle (= 0)$$

$$\begin{aligned}
\text{So, } & \boxed{E_n^{(2)} = \langle \psi_n^0 | H' | \psi_n^{(1)} \rangle} \\
&= \sum_{l=1} \langle \psi_n^0 | H' | \psi_l^0 \rangle \left[\frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_l^0} \right] \\
&= \sum_{l=1} \frac{\left| \langle \psi_n^0 | H' | \psi_l^0 \rangle \right|^2}{E_n^0 - E_l^0} \quad \text{, where } l \neq n
\end{aligned}$$

Wave Function $\rightarrow \psi_n^{(2)} = \sum_l b_l \psi_l^0$

By doing ket of equation 16.4 with $\langle \psi_n^0$

$$\langle \psi_m^0 |(16.4) \implies \langle \psi_m^0 | H' | \psi_n^{(1)} \rangle + \langle \psi_m^0 | H^0 | \psi_n^{(2)} \rangle = E_n^{(2)} \langle \psi_m^0 | \psi_n^0 \rangle + E_n^{(1)} \langle \psi_m^0 | \psi_m^{(1)} \rangle + \langle \psi_m^0 | E_n^0 | \psi_n^{(2)} \rangle$$

(= 0)

$$\implies \sum_{l=1}^{l \neq n} a_l \langle \psi_m^0 | H' | \psi_l^0 \rangle + \sum_l^{l \neq n} b_l E_m^0 \langle \psi_m^0 | \psi_l^0 \rangle = E_n^{(1)} \sum_l^{l \neq n} \langle \psi_m^0 | \psi_l^0 \rangle a_l + E_n^0 \sum_l^{l \neq n} b_l \langle \psi_m^0 | \psi_l^0 \rangle$$

$$\implies b_m (E_m^0 - E_n^0) = a_m E_n^{(1)} - \sum_l^{l \neq n} a_l \langle \psi_m^0 | H' | \psi_l^0 \rangle$$

$$\implies b_m = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} \frac{\langle \psi_n^0 | H' | \psi_n^0 \rangle}{(E_m^0 - E_n^0)} - \sum_l^{l \neq n} \frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_l^0} \frac{\langle \psi_m^0 | H' | \psi_l^0 \rangle}{E_m^0 - E_n^0}$$

$$\boxed{b_m = \sum_l^{l \neq n} \frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle \langle \psi_m^0 | H' | \psi_l^0 \rangle}{(E_n^0 - E_l^0)(E_n^0 - E_m^0)} - \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle \langle \psi_n^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)^2}} \tag{16.7}$$

16.2 page4-5

16.2.1 Anharmonic Oscillator

V(x) = $\frac{1}{2} m w^2 x^2 + b x^4$

So $H^o = -\frac{k^2}{2m} \nabla^2 + \frac{1}{2} m w^2 x^2$

and $H' = b x^4$

So $E_n^o = (n + \frac{1}{2}) \hbar \omega$

$\psi_n^o \rightarrow$ Hermit polynomials of harmonic oscillator

1^{st} order correction to ground state energy

$E_o^\omega = \langle 0 | b x^4 | 0 \rangle$ Now $x = x_o (a + a^+)^4$, $x_o = (\frac{\hbar}{2m\omega})^{\frac{1}{2}}$

$= b x^4 \langle 0 | (a + a^+)^4 | 0 \rangle$

$(a + a^+)$ can have 16 forms from $aaaa$ to $a^+ a^+ a^+ a^+$

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

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

The forms that have $a|0\rangle$ or $aaa^+|0\rangle$ have $\sqrt{n} = \sqrt{0} = 0$ so they have value of 0

The forms with different number of a and a+ like $aa^+a^+a^+|0\rangle = \#|2\rangle$ will not end with $|0\rangle$

They cannot be paired with $\langle 0|$ and are discarded

only 2 forms remain $\langle 0 | aa^+ aa^+ | 0 \rangle$ and $\langle 0 | aaa^+ a^+ | 0 \rangle$

$\langle 0|aa^+aa^+|0\rangle$

$=\sqrt{1} \qquad \langle 0|aa^+a|1\rangle$

$=\sqrt{1}\sqrt{1} \qquad \langle 0|aa^+|0\rangle$

$=\sqrt{1}\sqrt{1}\sqrt{1} \quad \langle 0|a|1\rangle$

$=\sqrt{1}\sqrt{1}\sqrt{1}\sqrt{1}\langle 0||0\rangle$

$=1$

$\langle 0|aaa^+a^+|0\rangle$

$=\sqrt{1} \qquad \langle 0|aaa^+|1\rangle$

$=\sqrt{1}\sqrt{2} \qquad \langle 0|aa|2\rangle$

$=\sqrt{1}\sqrt{2}\sqrt{2} \quad \langle 0|a|1\rangle$

$=\sqrt{1}\sqrt{2}\sqrt{2}\sqrt{1}\langle 0||0\rangle$

$=2$

so $E_o^\omega = (1+2)bx^4 = 3b(\frac{\hbar}{2m\omega})^2$

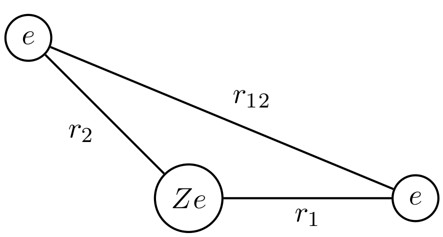
$E_o = E_o^o + E_o^\omega$

$E_o = \frac{1}{2}\hbar\omega + 3b(\frac{\hbar}{2m\omega})^2$

Griffiths book says

$\boxed{\langle\psi_n^o|bx^4|\psi_n^o\rangle = (6n^2+6n+3)b(\frac{\hbar}{2m\omega})^2}$

16.2.2 Ground State of Helium



Helium has 2 electrons at a distance r_1 and r_2 and the distance between them r_{12}

$H_1 = -\frac{\hbar^2}{2m}\vec{\nabla}_1^2 - \frac{Ze^2}{4\pi\epsilon_o r_1}$

$H_2 = -\frac{\hbar^2}{2m}\vec{\nabla}_2^2 - \frac{Ze^2}{4\pi\epsilon_o r_2}$

Total Hamiltonian Operator

$\text{H} = -\frac{\hbar^2}{2m}\vec{\nabla}_1^2 - \frac{Ze^2}{4\pi\epsilon_o r_1} + -\frac{\hbar^2}{2m}\vec{\nabla}_2^2 - \frac{Ze^2}{4\pi\epsilon_o r_2} + \frac{e^2}{4\pi\epsilon_o r_{12}}$

$\text{H} = H_1 + H_2 + H' \qquad [H_1 + H_2 = H^o]$

$H^o\psi_o^o(r_1, r_2) = E_{tot}^o\psi_o^o(r_1, r_2)$

$(H_1 + H_2)\psi^o(r_1)\psi^o(r_2) = (E^o + E^o)\psi^o(r_1)\psi^o(r_2)$ [$\psi^o(r_1)$ and $\psi^o(r_2)$ = Hydrogen wave function, $E^O = -Z^2 \times 13.6$]

ground state energy of H , E^O $(Z) = 1 = \frac{me^4}{8h^2\epsilon_o}$ $W_H = 13.6$ ev

So, $E^o_{tot} = -2Z^2W_H$

Correction term $E^1 = \iint \psi^o_1\psi^o_2 \frac{e^2}{4\pi\varepsilon_o r_{12}} \psi^o_1\psi^o_2 d\vec{r_1} d\vec{r_2}$.

$\psi^o_{n=1}(r_1) = 2(\frac{z}{a_o})^{3/2} e^{-\frac{Zr_1}{a_o}}$

$\psi^o_{n=1}(r_2) = 2(\frac{z}{a_o})^{3/2} e^{-\frac{Zr_2}{a_o}}$

$E^1 = 2^4 \frac{Z^6}{a_o^6} \times \frac{e^2}{4\pi\epsilon_o} \iint \frac{1}{r_{12}} exp[\frac{-2Z}{a_o} \ (r_1 + r_2)] \ d\vec{r_1} d\vec{r_2}$ $d\vec{r_i} = r_i^2 \sin\theta_i dr_i d\theta_i d\phi_i$

$= \frac{5}{4} ZW_H$

$E_{tot} = E^o_{tot} + E^1$

$E_{tot} = -2Z^2W_H + \frac{5}{4}ZW_H$

Chapter 17

Variational Method

Variation Method:

Ground state $E_1 \leq < H >$, where $< \Phi|H|\Phi >$

Trial Solution, $\Phi = e^{-\alpha r}$, $< \Phi|H|\Phi >$, $< H >= \frac{<\Phi|H|\Phi>}{<\Phi|\Phi>}$

with $H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{k}{r}$

$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}(r^2\frac{d}{dr}) = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}$

$$\begin{aligned}
\therefore < \Phi|H|\Phi > &= -\frac{\hbar^2}{2\mu}[< \Phi|\frac{d^2}{dr^2}|\Phi > + < \Phi|\frac{2}{r}\frac{d}{dr}|\Phi > - < \Phi|\frac{ke^2}{r}|\Phi >] \\
&= -\frac{\hbar^2}{2\mu}4\pi[\alpha^2[\int_0^\alpha r^2 e^{-2\alpha r}\, dr] + 2\alpha[\int_0^\alpha re^{-2\alpha r}\, dr] - k[\int_0^\alpha re^{-2\alpha r}\, dr]] \\
&= -\frac{\hbar^2}{2\mu}\left(\frac{\pi}{\alpha} - \frac{2\pi}{\alpha}\right) + \frac{k\pi}{\alpha^2} = \frac{\hbar\pi}{2\mu\alpha} + \frac{k\pi}{\alpha^2}
\end{aligned}$$

$$< \Phi|\Phi > = 4\pi[\int_0^\alpha r^2 e^{-2\alpha r}\, dr] = \frac{\pi}{\alpha^3}$$

$$\Longrightarrow < H > = \frac{\hbar^2\alpha^2}{2\mu} - k\alpha$$

$$\frac{\partial < H >}{\partial\alpha} = 0 \implies 2\alpha(\frac{\hbar^2}{2\mu}) = k \implies \boxed{\alpha = \frac{k\mu}{\hbar^2}}$$

$$\therefore E_{\min} = < H >_{\alpha = \frac{kr}{\hbar^2}} = \frac{\mu z^2 e^4}{32\pi^2{\epsilon_0}^2\hbar^2} \qquad , k = \frac{ze^2}{4\pi\epsilon_0}$$

continue...

$$\Phi_0 = \left(\frac{1}{\left(\frac{\pi}{\alpha_0}\right)^3}\right)^{1/2} e^{-\alpha_0 r} = \left(\frac{1}{\pi {a_0}^3}\right)^{1/2} e^{-\frac{r}{a_0}}$$

$$a_0 = \frac{\hbar^2}{k\mu} = \frac{\hbar^2(4\pi\epsilon_0)}{ze^2\mu} = \frac{1}{\alpha_0}$$

$$mv_0 a_0 = \hbar$$

$$\frac{m{v_0}^2}{a_0} = \frac{ze^2}{4\pi\epsilon_0 {a_0}^2}$$
$$\implies \frac{m\hbar^2}{{a_0}^3} = \frac{ze^2}{4\pi\epsilon_0 {a_0}^2}$$

$$\implies \boxed{a_0 = \frac{\hbar^2(4\pi\epsilon_0)}{ze^2 m}}$$

Harmonic Oscillator:

Trial Function Gaussian $\phi(x) = Ae^{-\alpha x^2}$

$$\phi(x) = Ae^{-\alpha x^2}$$

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

$$\langle\Phi|\Phi\rangle^{1/2} = A = \left(\frac{2\alpha}{\pi}\right)^{1/4}$$

$$\therefore \left\langle\phi|\hat{H}|\phi\right\rangle = \sqrt{\frac{2\alpha}{\pi}}\left[-2\alpha\int e^{-2\alpha x^2}dx + 4\alpha^2\int x^2 e^{-2\alpha x^2}dx\right] = -\alpha$$

Similarly $\left\langle\phi|x^2|\phi\right\rangle = \dfrac{1}{4\alpha}$

$$\langle H\rangle = \frac{\hbar^2\alpha}{2m} + \frac{1}{2}m\omega^2\left(\frac{1}{4\alpha}\right)$$
$$\langle H\rangle = \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha}$$

$$\frac{d}{d\alpha}\langle H\rangle = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha^2} = 0 \Rightarrow \alpha_0 = \frac{m\omega}{2\hbar}$$

$$\therefore \langle H\rangle_{\min} = \frac{\hbar^2}{2m}\alpha_0 + \frac{m\omega^2}{8\alpha_0} = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

$$\therefore \phi(x) = \left(\frac{2\alpha_0}{\pi}\right)^{1/4} e^{-\alpha_0 x^2}$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$$

Chapter 18

WKB method

$$\frac{d^2\Psi}{dx^2} + K^2\Psi = 0 \qquad K^2 = \frac{2m}{h^2}[E - V(x)]$$

V(x) is slowly varring

$$\rightarrow \Psi = \frac{A}{\sqrt{K}} exp\left(Ji\int K(x)dx\right) \qquad where\ E > V(x)$$

$$\rightarrow \frac{d^2\Psi}{dx^2} - \delta^2\Psi = 0 \qquad \delta = \frac{2m[V(x) - E]}{h^2} \qquad E < V(x)$$

$$\Psi = \frac{B}{\sqrt{\delta}} exp\left(J\int \delta dx\right) \qquad E > V(x)$$

Harmonic oscillator from WKB approximation
Classical turning point $V(x) = E_{tol}$

$$\frac{1}{2}m\omega^2 x^2 = E$$

$$\Rightarrow x = J\left(\frac{2E}{m\omega^2}\right)^{\frac{1}{2}} \longrightarrow x_1,\ x_2$$

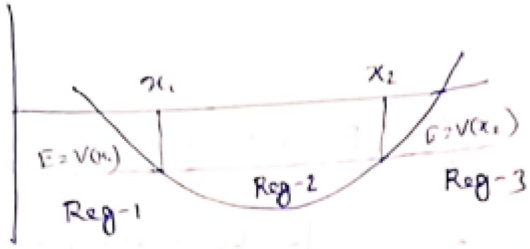
$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \Longrightarrow p = [2m\left(E - \frac{1}{2}m\omega^2 x^2\right)]^{\frac{1}{2}}$$

$$\int_{x_1}^{x_2} [2m(E - \frac{1}{2}m\omega^2 x^2)]^{\frac{1}{2}} dx = \left(n + \frac{1}{2}\right)\pi\hbar,\ n = 0, 1, 2, ...$$

$$Sin\theta = \left(\frac{m\omega^2}{2E}\right)^{\frac{1}{2}} x \Rightarrow cos\theta\ d\theta = \left(\frac{m\omega^2}{2E}\right)^{\frac{1}{2}} dx$$

$$\therefore \int_{-\frac{-\pi}{2}}^{\frac{\pi}{2}} (2mE)^{\frac{1}{2}} cos^2\theta \left(\frac{2E}{m\omega^2}\right)^{\frac{1}{2}} d\theta = \left(n + \frac{1}{2}\right)\pi\hbar$$

$$\left(\frac{2E}{\omega}\right)\frac{\pi}{2} = \left(n + \frac{1}{2}\right)\pi\hbar \Rightarrow E = \left(n + \frac{1}{2}\right)\hbar\omega$$



$$Reg-1 \Rightarrow \Psi_\beta = \frac{1}{\sqrt{r}} exp\left[-\int_{x2}^{x1} \delta dx\right] \qquad E < V(x)$$

$$For\ Region-1 \qquad E > V(x) : \Psi_1 = \frac{1}{\sqrt{\delta}} exp\left(\int_{x_1}^{x_2} \delta dx\right)$$

$$\delta^2 = \frac{2m\{V(x) - E\}}{\hbar^2}$$

$$For\ Region-2 \qquad E < V(x) : \Psi_2 = \frac{2}{\sqrt{K}} cos\left(\int_{x_1}^{x_2} Kdx - \frac{\pi}{4}\right) \qquad x_1 < x < x_2$$

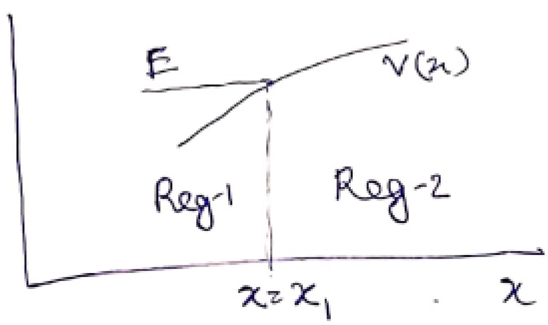
$$K^2 = \frac{2m[E - V(x)]}{\hbar^2}$$

$$modify\ \Psi_2 = \frac{2}{\sqrt{K}} cos\left(\int_{x_1}^{x_2} Kdx + \int_{x_2}^{x} Kdx - \frac{\pi}{4}\right)$$

$$\begin{aligned}
\Psi_2 &= cosA\ cosB + sinA\ sinB \\
&= cosA\ \left(-sin\left(\frac{-\pi}{2} + B\right)\right) + sinA\ \left(+cos\left(\frac{-\pi}{2} + B\right)\right) \\
&= \frac{-2}{\sqrt{K}}\ cos\left(\int_{x_1}^{x_2} Kdx\right)\ sin\left(\int_{x}^{x_2} Kdx - \frac{\pi}{4}\right) + \frac{2}{\sqrt{K}} sin\left(\int_{x_1}^{x_2} Kdx\right)\ cos\left(\int_{x}^{x_2} Kdx - \frac{\pi}{4}\right)
\end{aligned}$$

$$\int_{x_1}^{x_2} Kdx = \left(n + \frac{1}{2}\right)\pi \Rightarrow \boxed{\int_{x_1}^{x_3} Pdx = \left(n + \frac{1}{2}\right)\pi\hbar} \qquad \hbar K = p$$

Connection Formula



$$V(x)\ mean\ x = x_1, V(x) = V(x_1) + \frac{\delta V}{\delta x}_{x=x_1}(x - x_1)$$

$$\therefore \frac{d^2\Psi}{dx^2} + \cancel{V(x_1)\Psi} - \frac{2m}{\hbar^2}\left(\frac{\delta V}{\delta x}\right)_{x=x_1}(x-x_1)\Psi = \cancel{E\Psi}$$

Kramess Connection Formula

$$\frac{2}{K^{\frac{1}{2}}}\ cos\left(\int_x^{x_1} Kdx - \frac{\pi}{4}\right) \leftarrow \frac{1}{\delta^{\frac{1}{2}}}\ exp\left(-\int_{x_1}^{x} \delta dx\right)$$

$$\frac{1}{K^{\frac{1}{2}}} sin\left(\int_x^{x_1} Kdx - \frac{\pi}{4}\right) \rightarrow -\frac{1}{\delta^{\frac{1}{2}}}\ exp\left(\int_{x_1}^{x_2} \delta dx\right)$$