I. Introduction

Quantum Mechanics is the physics of matter at scales much smaller than we are able to observe of feel. In another definition, a Quantum Mechanics is one of the more sophisticated field in physics that has affected our understanding of Nano-meter length scale systems important for chemistry, materials, optics, and electronics. The existence of orbitals and energy levels in atoms can only be explained by quantum mechanics. Quantum mechanics can explain the behaviors of insulators, conductors, semi-conductors, and giant magneto-resistance. It can explain the quantization of light and its particle nature in addition to its wave nature. Quantum mechanics can also explain the radiation of hot body, and its change of color with respect to temperature. It explains the presence of holes and the transport of holes and electrons in electronic devices.
Quantum mechanics has played an important role in photonics, quantum electronics, and micro-electronics.

II. Principles of Quantum Mechanics

1.Black body radiation

A. Classical Theory (Rayleigh –Jeans formula)

- A black body is an object that is a perfect absorber of radiation. In the ideal case, it absorbs all of the light that falls on it, no light is reflected by it, and no light passes through it. While such on object doesn't reflect any light, if we heat up a black body, it can radiate light.
- The Rayleigh –Jeans formula has been used to give the black body radiation energy density:

$$u = \begin{pmatrix} number\ of\ degree\ of \\ freedom\ for\ frequency\ \nu \end{pmatrix} \begin{pmatrix} average\ energy\ per \\ degree\ of\ fredom \end{pmatrix}$$

Using classical physics, the average energy per degree of freedom can be calculated in the following way. Let's call the energy E, Boltzmann's constant k.

$$\bar{E} = \frac{\int_0^\infty E e^{-E/kt} dE}{\int_0^\infty e^{-E/kt} dE} = \frac{(kT)^2}{kT}$$

Using classical theory, the number of degrees of freedom per frequency was found to be:

$$\frac{8\pi\nu^2}{c^3}$$

All together the Rayleigh –Jeans formula tells us that the energy density is:

$$u(\nu, T) = \left(\frac{8\pi\nu^2}{c^3}\right)(kT)$$

Where ν is the frequency of radiation emitted, c speed of light in vacuum, and T the black body temperature.

- We can see from this formula that as ν gets large, it's going to blow sky-high.
- Worse—if you integrate over all frequencies to get the total energy per unit volume, you will get infinity. The formula only works at low frequencies.

- Obviously, this is not what is observed experimentally, and the predication that the energy at high frequencies would go to infinity became known as the "ultraviolet catastrophe" (since ultraviolet is light of high frequency).
- The formula is computed using integration, which means that it has been assumed that energy exchange is *continuous*. What if instead, only certain fixed values of energy exchange was allowed?

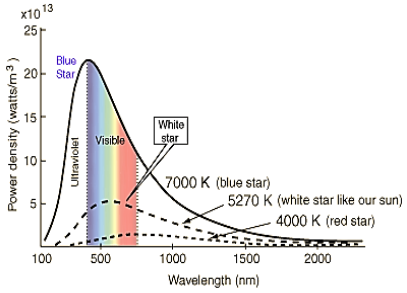
B. Quantum Theory (Planck's Formula)

- A practical blackbody is made of a metallic cavity with a small hole through which radiation can escape.
- Planck mades the assumption that an exchange of energy between the electrons in the wall of the cavity and electromagnetic radiation can only occur in discrete amounts.
- The first consequence of this assumption is that the integrals above turn into discrete sums. we must change all integrals to sums:

$$\int \Rightarrow \sum$$

- The second important piece of data that Planck told us, was that energy comes in little bundles, that we will call the basic "quantum of energy." According to Planck, the basic quantum of energy ε is given by:

$$\varepsilon = h\upsilon$$



Furthermore, energy can only come in amounts that are integer multiples of the basic quantum:

$$E = nh\upsilon, \qquad n = 0,1,2, \ldots.$$

The constant $h = 6.62 \times 10^{-34}$ (Joules-seconds) is called *Planck's constant*. It is frequently convenient to use the symbol $\hbar = h/2\pi$

- Incorporating this assumption with the change from integrals to discrete sums, we now have:

$$\bar{E} = \frac{\sum_{n=0}^{\infty} n\varepsilon e^{-n\varepsilon/kT}}{\sum_{n=0}^{\infty} e^{-n\varepsilon/kT}} = \frac{h\nu}{e^{h\nu/kT} - 1}$$

To get the complete Planck formula for blackbody radiation, we just substitute this term for kT in the Rayleigh-Jeans law. The exponential in the denominator decays much faster than ν^2. The net result is that the average energy term cuts off any energy density at high frequencies. The complete Planck formula for the energy density of blackbody radiation is:

$$u(\nu, T) = \left(\frac{8\pi\nu^2}{c^3}\right)\left(\frac{h\nu}{e^{h\nu/kT} - 1}\right)$$

- As a conclusion, Planck postulated in1900 that thermal radiation emitted from a heated surface is in a form of discrete packets of energy called quanta.

2. Einstein interpretation for photoelectric effect:

- In 1905, Einstein suggested the energy in a light wave is also contained in discrete packets or bundles.
- The particle -like packet of energy is called photon, whose energy is given by

$$E = h\upsilon$$

And linear momentum

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

Where λ is the wavelength of the light wave. Using the relation $c = \upsilon\lambda$, we can rewrite the momentum of a photon as:

$$p = \frac{h}{\lambda} = \frac{h}{c/\upsilon} = \frac{h}{c(h/E)} = \frac{E}{c}$$

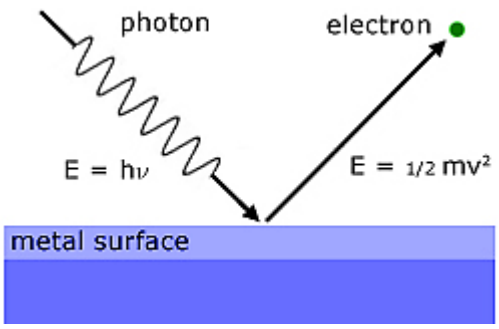
- The photoelectric effect process involves the emission of electrons from a metal when light strikes the surface. The maximum energy of the emitted electrons is found to be:

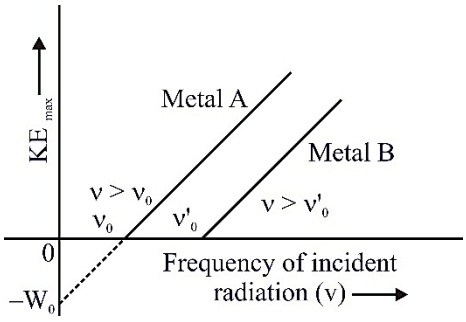
$$qV_o = E_{max}$$

Where q is the charge of the electron and V_o is the *stopping potential*.

- The minimum energy required to remove an electron is called the work function of the material and any access photon energy goes into kinetic energy of the photoelectron.

$$K.E = T_{max} = \frac{1}{2}mv^2 = h\upsilon - h\upsilon_o. \quad Work\ function = h\upsilon_o$$





Each metal has a characteristic threshold frequency υ_o such that:

$$qV_o = h\upsilon - h\upsilon_o$$

The ideas of Planck and Einstein can be summarized by the Planck-Einstein relations.

The Planck-Einstein Relations

The Planck-Einstein relations connect the particle-like properties of energy and momentum to wavelike properties of frequency and wave vector k. Recalling that frequency $\nu = \omega/2\pi$.

$$E = h\upsilon = \hbar\omega$$
$$p = \hbar k$$

3.The Bohr Theory of the Atom

In 1913, Bohr tells us that like Planck's blackbody oscillators, atoms can exchange energy only in fixed discrete amounts. Neils Bohr noticed this and proposed two radical ideas about the behavior of electrons in atoms.

Bohr Makes Two Key Assumptions About the Atom

1. An electron can only orbit about the nucleus in such a way that the orbit is defined by the relationship:

$$mvr = n\hbar, \qquad n = 1, 2, \ldots$$

where v is the velocity of the electron, r is the radius of the orbit, and m is the mass of the electron. The presence of n in the formula restricts the angular momentum of the electron to integer multiples of $\hbar$, where the angular momentum is given by:

$$L = n\hbar$$

2. Electrons only radiate during transitions between states. A transition from energy state E_i to energy state E_f is accompanied by the emission of a photon of energy:

$$h\nu = E_i - E_f$$

The Coulomb force between the positively charged nucleus and the negatively charged electron is what keeps the electrons in orbit. Setting this equal to the centrifugal force:

$$\frac{e^2}{r} = \frac{mv^2}{r}$$

Results in the following expressions for the velocity of the electron and the radius of the orbit. We label each quantity with subscript n to conform with assumption (a) above:

$$v_n = \frac{e^2}{n\hbar} \quad \text{(Velocity of electron in orbit } n\text{)}$$

$$r_n = \frac{n^2\hbar^2}{me^2} \quad \text{(Radius of orbit } n\text{)}$$

Example 1.

Derive the energy of an electron in the hydrogen atom using Bohr's formulas.

Solution:

We start by recalling that the

$$total\ energy = kinetic\ energy + potential\ energy = T + V$$

For an electron moving in the Coulomb potential of a proton, the potential is just

$$V = -\frac{e^2}{r}$$

Using the formula for the radius of orbit n this becomes:

$$V = -\frac{e^2}{r_n} = -\frac{e^2}{n^2\hbar^2}me^2 = -\frac{me^4}{n^2\hbar^2}$$

For the kinetic energy, we obtain:

$$T = \frac{1}{2}mv_n^2 = \frac{1}{2}m\left(\frac{e^2}{n\hbar}\right)^2 = \frac{me^4}{2n^2\hbar^2}$$

The total energy of an electron in orbit n is therefore:

$$E_n = T_n + V_n = \frac{me^4}{2n^2\hbar^2} - \frac{me^4}{n^2\hbar^2} = -\frac{me^4}{2n^2\hbar^2} = -\frac{2\pi^2me^4}{n^2h^2}$$

Example 2:

Derive a relation that predicts the frequencies of the line spectra of hydrogen.

Solution:

Bohr proposed that the frequency of a photon emitted by an electron in the hydrogen atom was related to transitions of energy states as:

$$h\nu = E_i - E_f$$

The energy of state n is:

$$E_n = -\frac{2\pi^2 me^4}{n^2 h^2}$$

Therefore:

$$E_i - E_f = -\frac{2\pi^2 me^4}{n_i^2\, h^2} + \frac{2\pi^2 me^4}{n_f^2\, h^2} = \frac{2\pi^2 me^4}{h^2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

Putting this together with Bohr's proposal we find the frequency is:

$$\nu = \frac{E_i - E_f}{h} = \frac{2\pi^2 me^4}{h^3}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

This formula can be used to predict the line spectra of hydrogen.

4.De Broglie Hypothesis (Wave particle duality)

- In 1923 Louis de Broglie proposed that the Planck-Einstein relations should be extended to material particles.
- The reasoning that led de Broglie to put forward his revolutionary hypothesis runs as follows. The entire physical universe is composed of matter and radiation. In quantum theory of radiation, a fragment or quantum of energy E is assigned a frequency, $\omega\ (= 2\pi\nu)$ such that $E = h\nu$, or a particle with energy E is associated with a wave of frequency $\omega = E/\hbar$.
- In addition, momentum is related to the wave vector via:

$$p = \hbar k$$

- Applying these simple relations to material particles like electrons, de Broglie proposed that a material particle moving with momentum p has a wavelength:

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

- From this notion de Broglie speculated that material particles, which are also fragment of energy ($E = mc^2$), might be assigned some characteristic frequency. A material particle of rest mass m_o is equivalent to energy $m_o c^2$, therefore, according to de Broglie idea we can write

$$m_o c^2 = \hbar\omega$$

Where ω, is the frequency of some intrinsic periodic process that associated with the material particle; Let us see what this periodic process appears to an observer with respect to which it is moving.

- The light wave in the photoelectric effect behave as if they are particle.
- In 1924, De Broglie postulated the existence of matter wave. Since wave exhibit particle-wave behavior, then particle should be expected to show particle-wave properties.

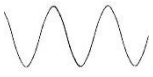


Energy $E = \frac{1}{2}mv^2$

Momentum $\vec{p} = m\vec{v}$

E-p relation $E = \frac{p^2}{2m}$

Force $F = ma = m\frac{d^2}{dt^2}$



Energy $E = h\nu = \hbar w$

Wavelength $\lambda = \frac{c}{\nu}$

Wavelength of particle $\lambda = \frac{h}{\sqrt{2mE}}$

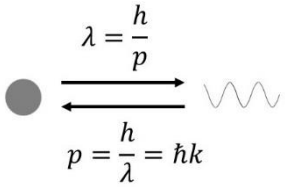
Wave equation $\frac{\partial^2}{\partial x^2}\Psi(x.t) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Psi(x.t)$

- Wave particle duality principle

Particle: momentum ⇒ wavelength
Wave: wavelength ⇒ momentum

The momentum of photon $p = \frac{h}{\lambda} = \hbar k.$ $\left(\hbar = \frac{h}{2\pi}.\ k = \frac{2\pi}{\lambda}\right).$

The wavelength of particle $\lambda = \frac{h}{p}$, (*De Broglie wavelength*)**.**



Example 3:

A thermal neutron has a speed *v* that corresponds to room temperature *T* = 300 K. What is the wavelength of a thermal neutron?

Solution:

At temperature T average energy is:

$$\bar{E} = \frac{3}{2}KT$$

Where k is Boltzmann's constant. By equating the kinetic energy to this quantity with T = 300 K, we can find the momentum of the neutron:

$$\frac{p^2}{2m_n} = \frac{3}{2}KT$$

Using de Broglie's relation, we obtain the wavelength of the thermal neutron:

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{3m_nKT}} = \frac{6.63 \times 10^{-34}}{\sqrt{3(1.67 \times 10^{-27})(1.38 \times 10^{-23})(300)}} = 1.4\ A^{\circ}$$

III. Special Relativity

- Lorentz Factor γ: is the factor by which time, length, and relativistic mass change for an object while that object is moving. $\gamma = 1/\sqrt{1 - \frac{v^2}{c^2}}$.
- Relativistic mass m_o: the mass of an object m in motion is dependent on γ and the rest mass m_o; $m = m_o\gamma$
- Relativistic momentum: is classical momentum multiplied by the Lorentz factor γ.

$$\vec{p} = \gamma m_o\vec{v}, \qquad \lambda = \frac{h}{p} = \frac{h}{\gamma m_o v} = \frac{h}{m_o v}\sqrt{1 - \frac{v^2}{c^2}}$$

- Relativistic Energy (rest energy): is Einstein's famous equation by the Lorentz factor γ.

$$E = \gamma mc^2 = \gamma m_o c^2, \ \ \nu = \frac{E}{h} = \frac{\gamma m_o c^2}{h} = \frac{m_o c^2}{h}\Big/\sqrt{1 - \frac{v^2}{c^2}}$$

Einstein's famous equation ($E = mc^2$) tells us that mass another form of energy, which means mass can be converted into energy and vice versa.

1. Relation between Energy and Momentum

Using the Newtonian definitions of energy and momentum $E = \frac{1}{2}mv^2$ and $p = mv$, we can find $E = \frac{p^2}{2m}$

Now consider the relativistic definitions

$$E = \gamma mc^2$$
$$p = \gamma mv$$
$$p^2 = \gamma^2 m^2 v^2$$
$$p^2c^2 = \gamma^2 m^2 v^2 c^2 = \gamma^2 m^2 c^4 \frac{v^2}{c^2} = \gamma^2 m^2 c^4 \left(1 - \frac{1}{\gamma^2}\right)$$
$$p^2c^2 = \gamma^2 m^2 c^4 - m^2 c^4$$

But $$E = \gamma mc^2$$

So $$p^2c^2 = E^2 - m^2c^4$$

Thus, equivalent relationship between energy and momentum in Relativity is:

$E^2 = p^2c^2 + m^2c^4$ or equivalently $m^2c^4 = E^2 - p^2c^2$

2.Special case of the energy-momentum relation in relativity

1. If the body is a massless particle ($m_o = 0$) then $E = Pc$ for photon.
2. If the body speed v is much less than c so that $E^2 = \frac{1}{2}m_o v^2 + m_o^2 c^4$ the body total energy is simply its classical kinetic energy plus its rest energy.
3. If the body is its rest ($v = 0$) in center of momentum frame ($p = 0$) we find $E = E_o$ and $m = m_o$.

IV. De Broglie Hypothesis (Matter Wave)

- All matter can exhibit wave like behavior, example; a beam of electrons can be diffracted like a beam of light or water wave.
- Max Planck proposed that light is emitted in discrete quanta of energy; example; black body thermal radiation.
- Planck-Einstein relation; $E = h\nu$; E-P relation $p = \frac{E}{c} = \frac{h}{\lambda}$.
- De Broglie relations

$$\lambda = \frac{h}{p}, \qquad \nu = \frac{E}{h}$$
$$p = \hbar k, \qquad E = \hbar\omega$$

- Group velocity of the wave is equal to the particle's speed corresponding.

$$v_g = \frac{\partial w}{\partial k} = \frac{\partial (E/\hbar)}{\partial (p/\hbar)} = \frac{\partial E}{\partial p}$$

i.For free non-relativistic particle.

$$v_g = \frac{\partial E}{\partial p} = \frac{\partial}{\partial p}\left(\frac{p^2}{2m}\right) = \frac{p}{m} = \frac{mv}{m} = v$$

ii.For free relativistic particle in special relativity

$$v_g = \frac{\partial E}{\partial p} = \frac{\partial}{\partial p}\left(\sqrt{p^2c^2 + m^2c^4}\right) = \frac{pc^2}{\sqrt{pc^2 + m^2c^4}} = \frac{pc^2}{E}$$

According to the phase velocity $v_p = \frac{E}{p} = \frac{c^2}{v}$

$$v_g = \frac{pc^2}{E} = \frac{c^2}{v_p} = \frac{c^2}{\frac{c^2}{v}} = v$$

- Phase velocity of the wave is equal to the product of the particle's frequency and its wavelength.
- Phase velocity of particle also behave as wave with complex phase.

$$v_p = \frac{w}{k} = \frac{E/\hbar}{p/\hbar} = \frac{E}{p}$$

Using the relativistic relation for energy and momentum

$$v_p = \frac{E}{p} = \frac{mc^2}{mv} = \frac{\gamma m_o c^2}{\gamma m_o v} = \frac{c^2}{v}$$

- The particle speed $v < c$ for any object that has mass (acorrding to special relativity).
- The phase velocity of matter waves exceeds c , i.e. $v_p > c$, this mean it approach c when the particle speed is the relativistic range.
- The superluminal (Faster than Light) phase velocity does not violet special relativity, because phase propagation carries no energy.
- For example, Electron energy packet that is moving with velocity v, that its frequency was apparently reduce to $\nu = \nu_o\sqrt{1 - \frac{v^2}{c^2}}$ Then $\lambda\nu = \frac{E}{p} = v_p$.

V.The theory of quantum mechanics

- Schrödinger and Heisenberg proposed works only for nonrelativistic phenomena, which called nonrelativistic quantum mechanics.
- Dirac succeeded (1928) in extending quantum mechanics to realm of relativistic quantum mechanics. This theory predicted the existence of a new particle "Positron (e^+) , $antielectron$ ".
- Pair production (photon→ $e^- + e^+$).
- All the microscopic particles level, however, the waves associated with material particles are the same size or exceed the size of system.

1.Particle versus waves

A. Classical view of particles and waves

- In classical physics: particles and waves are mutually exclusive; they exhibit completely different behavior.
- The full description of a particle requires only one parameter, the position vector $x(\vec{r})$.

- The complete description of a wave requires two parameters; the amplitude and the phase.
- 3-D plane waves can be described by the wave function $\psi(\vec{r},t)$;

$$\psi(\vec{r},t) = Ae^{i(k.\vec{r}-\omega t)} = Ae^{i\phi}$$

A: Amplitude and ϕ:Phase.

- The intensity of the wave is given by $I = |\ \psi(\vec{r},t)|^2$.

B. Quantum view of particles and waves

- The interference pattern obtained from the double slit experiment indicates that electrons display both particle and wave propagation behavior.
- When electron observed or detected one by one they behave like particles, but when they are detected after many measurements (distribution of the detected electrons) they behave like wave of wavelength $\left(\lambda = \frac{h}{p}\right)$ and display an interference pattern.

2.Indeterministic Nature of Microphysical world (Predictability and Determinacy)

- Waves are not localized in space.
- Heisenberg postulates the indeterministic nature of microphysical world.
- Born introduced the probabilistic interpretation of quantum mechanics.

Heisenberg uncertainty principle

A. Classically

- Initial position $x_o(\vec{r})$ and velocity $v_o(\vec{r})$ can be determined.
- Force acts on particle by means of Newton's second law, so that, we can determine $x_o(\vec{r})$ and $v_o(\vec{r})$ with completely deterministic.

B. Quantumly

- Wave function (particle's wave) cannot be localized in microphysical system.
- According to Heisenberg principle; if the momentum p_x in x-direction for particle is measured with uncertainty, then its position x in x-direction at the same time cannot be measured accurately then $\Delta x = \frac{\hbar}{2\Delta p_x}$.
- In 3D $\Delta x\Delta p_x \geq \frac{\hbar}{2}$, $\Delta y\Delta p_y \geq \frac{\hbar}{2}$, $\Delta z\Delta p_z \geq \frac{\hbar}{2}$ and $\Delta E\Delta t \geq \frac{\hbar}{2}$

So that the probabilistic is good answer to determine position and momentum.

3.Probabilistic Interpretation

- In Q.M. $\psi(\vec{r},t)$ describing the wave properties of a particle.
- The wave intensity I associated in quantum effect with $|\ \psi(\vec{r},t)|^2$.
- The intensity of a wave at a given point in space is proportional to the probability of finding it at the point.
- In 1927 Born interpreted $|\ \psi(\vec{r},t)|^2$ as the probability density.
- In probability $d\mathrm{P}(\vec{r},t)$ of finding a particle at time t in the volume element d^3r located between r and $r + dr$, and can be written as

$$d\mathrm{P}(\vec{r},t) = |\ \psi(\vec{r},t)|^2 d^3r$$

- In all space the probability of finding a particle is equal one

$$\int_{all\ space} |\ \psi(\vec{r},t)|^2 d^3r = 1$$

4.Wave packets

A. In classical physics;

A particle is well localized in space, for its position and velocity can be calculated simultaneously to arbitrary precision.

B. In Quantum mechanics;

- Q.M. describes a material particle by a wave function corresponding to matter wave associated with the particle (de Broglie conjecture).
- A particle is localized within a certain region of space can be described by matter wave whose amplitude is large in that region and zero outside it.; Therefore, a wave matter must be localized around the region of space within which the particle is confined.
- A localized wave function is called a wave packet. A wave packet therefore consist of a group velocity of waves of slightly different wavelengths with phase and amplitudes so chosen that they interfere constructively over a small region of space and destructively elsewhere.

i. Localized wave packets

- Localized wave packets can be constructed by superposing in the same region of space, waves of slightly different of wavelengths, but with phases and amplitudes chosen to make the superposition constructive in the desired region and destructive outside it.
- We can construct the packet $\psi(x,t)$ by superposing planes waves (propagation along the x-axis) of different frequencies (or wavelengths)

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \emptyset(k)\, e^{i(kx-\omega t)}\mathrm{dk}; \qquad (1)$$

$\emptyset(k)$ is the amplitude of the wave packet.

- It $t = 0$, Localized wave packets in 1D $\psi(x,0)$ can be write as $\psi_o(x)$:

$$\psi_o(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \emptyset(k)\, e^{ikx} dk; \qquad (2)$$

Fourier transform can be used to find the amplitude value $\emptyset(k)$ of wave packet.

$$\emptyset(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \psi_o(x)\, e^{-ikx} dx; \qquad (3)$$

- $|\psi_o(x)|$ peaks at $x = 0$ and vanishes far away from $x = 0$. On the one hand, as $x \to 0$ we have $e^{ikx} \to 1;$ hence the waves of different frequencies interfere constructively. (i.e. the various k- integrations (2) add constructively).
  On other hand, far away from $x = 0$ (i.e., $|x| \gg 0$) the phase e^{ikx} goes through many periods leading to violent oscillations, thereby yielding destructive interference (i.e., the various k- integrations (2) add up to zero).
- The same comments apply to amplitude $\emptyset(k)$ as well; $\emptyset(k)$ peaks at $k = 0$ and vanish far away.

- The physical interpretation of wave packet is obvious: $\psi_o(x)$ is the wave function or probability amplitude for finding the particle at position $x = 0$, hence $|\psi_o(x)|^2$ gives the probability density for finding particle at x, and $P(x)dx = |\psi_o(x)|^2 dx$ gives the probability of finding the particle between x and $x + dx$.
- The physical interpretation of $\emptyset(k)$ can be found from eqs. (2) and (3) as follows:

$$\int_{-\infty}^{+\infty} |\psi_o(x)|^2 dx = \int_{-\infty}^{+\infty} |\emptyset(k)|^2 dk$$

Then if $\psi_o(x)$ is normalized so is $\emptyset(k)$ and vice versa.

- The function $\emptyset(k)$ can be interpreted as a probability amplitude for measuring a wave vector for a particle in the state $\emptyset(k)$.
- Moreover, while $|\emptyset(k)|^2$ represents the probability density for measuring k as the particle's wave vector, the quentity $P(k)dk = |\emptyset(k)|^2 dk$ gives the probability of finding the particle's wave vector between k and $k + dk$.
- We can extract information about the particle's motion by simply expressing its corresponding matter wave in terms of the particle's energy, E, and momentum, p.
- Using $k = p/\hbar, dk = dp/\hbar,\ E = \hbar\omega$ and redefindining $\tilde{\emptyset}(p) = \emptyset(k)/\sqrt{\hbar}$, we can write (1) to (3) as follows:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \tilde{\emptyset}(p)\, e^{i(px-Et)/\hbar} \mathrm{dp}; \qquad (4)$$

$$\psi_O(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \tilde{\emptyset}(p)\, e^{ipx/\hbar} \mathrm{dp}; \qquad (5)$$

$$\tilde{\emptyset}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi_O(x)\, e^{-ipx/\hbar} \mathrm{dx}; \qquad (6)$$

Where $E(p)$ is the total energy of the particle described by the wave packet $\psi(x,t)$ and $\tilde{\emptyset}(p)$ is the momentum amplitude of the packet.

Example 4: Gaussian and space wave packets

(a) Find $\psi_o(x,0)$ for a Gaussian wave packet $\emptyset(k) = A\, exp[-a^2\,(k-k_o)^2/4]$, where A is a normalization factor to be found. Calculate the probability to find the particle in the region $-a/2 \le x \le a/2$.

(b) Find $\emptyset(k)$ for a square wave packet $\psi_O(x) = \begin{cases} Ae^{ik_o x} & |x| \le a \\ 0, & |x| > a. \end{cases}$

Find the factor A so that $\psi(x)$ is normalized.

Solution:

(a) The normalization factor A is easy to obtain:

$$1 = \int_{-\infty}^{+\infty} |\emptyset(k)|^2 dk = |A|^2 \int_{-\infty}^{+\infty} exp\left[-\frac{a^2}{2}(k-k_o)^2\right] dk$$

Using $z = k - k_o$, and $\int_{-\infty}^{+\infty} exp\left[-\frac{a^2 z^2}{2}\right] dz = \frac{\sqrt{2\pi}}{a}$, sothat $|A|^2 \sqrt{\frac{2\pi}{a^2}} = 1$

$\therefore$ $$A = \sqrt{\frac{a}{\sqrt{2\pi}}} = \left(\frac{a^2}{2\pi}\right)^{1/4}$$

The wave packet corresponding to

$$\emptyset(k) = \left(\frac{a^2}{2\pi}\right)^{1/4} exp\left[-\frac{a^2}{4}(k-k_o)^2\right]$$

Is

$$\psi_o(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \emptyset(k)\, e^{ikx} dk = \frac{1}{\sqrt{2\pi}}\left(\frac{a^2}{2\pi}\right)^{1/4}\int_{-\infty}^{+\infty} e^{-a^2(k-k_o)^2/4+ikx}\, dk$$

To finish the integration. We need simply to arrange the exponent's argument as follow:

$$-\frac{a^2}{4}(k-k_o)^2 + ikx = -\left[\frac{a}{2}(k-k_o) - \frac{ix}{a}\right]^2 - \frac{x^2}{a^2} + ik_o x$$

The introduction of new variable $y = \frac{a}{2}(k-k_o) - \frac{ix}{a}$ yields $dk = \frac{2dy}{a}$

Substitute this variable in the function of the wave packet, this leads to

$$\psi_o(x) = \frac{1}{\sqrt{2\pi}}\left(\frac{a^2}{2\pi}\right)^{1/4}\int_{-\infty}^{+\infty} e^{-x^2/a^2} e^{ik_o x} e^{-y^2}\left(\frac{2}{a}dy\right)$$

$$= \frac{1}{\sqrt{\pi}}\left(\frac{2}{\pi a^2}\right)^{1/4} e^{-x^2/a^2} e^{ik_o x}\int_{-\infty}^{+\infty} e^{-y^2}\, dy$$

Since $\int_{-\infty}^{+\infty} e^{-y^2}\, dy = \sqrt{\pi}$, the expression become

$$\psi_o(x) = \left(\frac{2}{\pi a^2}\right)^{1/4} e^{-x^2/a^2} e^{ik_o x},$$

Where $e^{ik_o x}$ is the phase of $\psi_o(x)$.

$\psi_o(x)$ is an oscillating wave with wave numberk_o modulated by a Gaussian envelope centered at the origin. The wave function $\psi_o(x)$ is complex.

The probability of finding the particle in region $-a/2 \le x \le a/2$ can be obtained at once from the wave packet above:

$$\mathrm{P} = \int_{-a/2}^{a/2} |\psi_o(x)|^2\, dx = \sqrt{\frac{2}{\pi a^2}}\int_{-a/2}^{+a/2} e^{-x^2/a^2}\, dx = \frac{1}{\sqrt{2\pi}}\int_{-1}^{+1} e^{-z^2/2}\, dz \cong \frac{2}{3},$$

Where we have used the change of variable $z = 2x/a$.

(b) The normalization of $\psi_o(x)$ is straightforward:

$$1 = \int_{-\infty}^{+\infty} |\psi_o(x)|^2 dx = |A|^2\int_{-a}^{+a} e^{-ik_o x} e^{ik_o x} dx = |A|^2\int_{-a}^{+a} dx = 2a\,|A|^2;$$

Hence $A = 1/\sqrt{2a}$, the Fourier transform of $\psi_o(x)$ is:

$$\emptyset(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \psi_o(x)\, e^{-ikx} dx = \frac{1}{2\sqrt{\pi a}}\int_{-a}^{+a} e^{ik_o x} e^{-ikx} dx = \frac{1}{\sqrt{\pi a}}\frac{sin(k-k_o)a}{k-k_o}$$

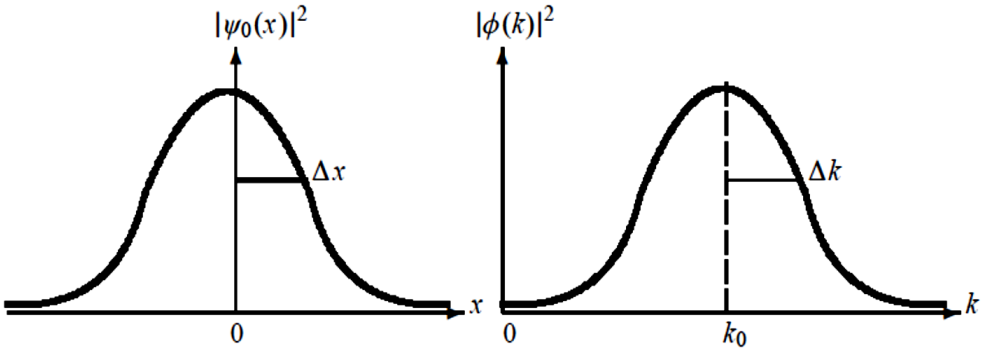


Figure: Two localized waves packets: $\psi_o(x) = (2/\pi a^2)^{1/4} e^{-x^2/a^2} e^{ik_o x}$ and $\emptyset(k) = (a^2/2\pi)^{1/4} e^{-a^2(k-k_o)^2/4}$;they peak at $x = 0$ and $k = k_o$,respectively, and vanish far away.

ii. Wave packets and the Uncertainty principle

- The width of wave packet $\psi_O(x)$ and the width of its amplitude $\emptyset(k)$ are not independent, they are correlated by a reciprocal relationship. As it turns out, the reciprocal relationship between the width in the x and k space has direct connection to Heisenberg uncertainty relation.
- Let us illustrate the main ideas on the Gaussian wave packet treated in the previous example.

$$\psi_o(x) = \left(\frac{2}{\pi a^2}\right)^{1/4} e^{-x^2/a^2} e^{ik_o x}, \quad \emptyset(k) = \left(\frac{a^2}{2\pi}\right)^{1/4} exp\left[-\frac{a^2}{4}(k-k_o)^2\right]$$

As display in Figure above, $|\psi_o(x)|^2$ and $|\emptyset(k)|^2$ are centered at x=0 and $k = k_o$, respectively.

It is convenient to define half-widths Δx and Δk as corresponding to the half-maxima of $|\psi_o(x)|^2$ and $|\emptyset(k)|^2$.

When x varies from 0 to $\pm\Delta x$ and k from k_o to $k_o \pm \Delta k$ the functions $|\psi_o(x)|^2$ and $|\emptyset(k)|^2$ drop to $e^{-1/2}$:

$$\frac{|\psi(\pm\Delta x,0)|^2}{|\psi(0,0)|^2} = e^{-1/2}, \frac{\left|\emptyset\left(\begin{matrix}k_o\pm\\ 0\Delta k\end{matrix}\right)\right|^2}{|\emptyset(k_o)|^2} = e^{-1/2}$$

These equations, combined with $\psi_o(x)$ and $\emptyset(k)$ leads to $e^{-2\Delta x^2/a^2} = e^{-1/2}$ and $e^{-a^2\Delta k^2/2} = e^{-1/2}$, respectively, or to

$$\Delta x = \frac{a}{2}, \qquad \Delta k = \frac{1}{a},$$

Hence $\Delta x \Delta k = \frac{1}{2}$, Since $\Delta k = \frac{\Delta p}{\hbar}$ we have $\Delta x \Delta p = \frac{\hbar}{2}$.

The relation shows that if the packet's width is narrow in x-space, its width momentum space must be very board, and vice versa.

The Gaussian wave packet is called *minimum uncertainty* wave packet.

The value of the uncertainty product $\Delta x \Delta p$ varies with the choice of ψ, but the lowest bound $\hbar/2$, is provided by a Gaussain wave function.

iii. Motion of wave packets (Propagation of a wave packet without Distortion)

- The angular frequency ω is proportional to the wave number k, this case corresponds to *nondispersive* propagation.
- Since the constant of proportionality has the dimension of a velocity v_o, which we denote by (i.e. $\omega = v_o k$), the wave packet becomes:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \emptyset(k)\, e^{ik(x-v_o t)} \mathrm{dk};$$

So that $\psi(x,t) = \psi(x - v_o t)$.

Therefore, when ω is proportional to k ,so that $\omega = v_o k$, the wave packet travls to the right with constant velocity *without distortion*.

- We are interested in the wave packets that describe particle. Therefore, we need to consider the more general case of *dispersive* media which transmit harmonic waves of different frequencies at different velocities.
- This means ω that is a function of k: $\omega = \omega(k)$.
- The amplitude $\emptyset(k)$ peaks at $k = k_o$, then $\emptyset(k) = g(k - k_o)$ is appreciably different from zero only in a narrow range $\Delta k = k - k_o$.
- We can Taylor expand $\omega(k)$ about k_o as:

$$\omega(k) = \omega(k_o) + (k - k_o)\frac{d\omega(k)}{dk}\Big|_{k=k_o} + \frac{1}{2}(k - k_o)^2 \frac{d^2\omega(k)}{dk^2}\Big|_{k=k_o} + \cdots$$
$$= \omega(k_o) + (k - k_o)v_g + (k - k_o)^2\alpha + \cdots$$

Where $v_g = \frac{d\omega(k)}{dk}\Big|_{k=k_o}$ and $\alpha = \frac{1}{2}\frac{d^2\omega(k)}{dk^2}\Big|_{k=k_o}$

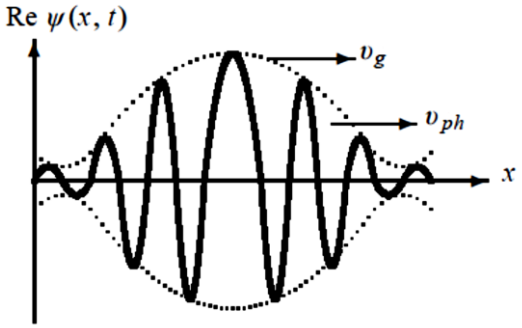


Figure: The function $Re\ \psi(x,t)$ of the wave packet represented here by solid curve contained in the dashed –curve envelope, propagate with *group* velocity v_g along the x-axis, move with the different *phase* velocities v_{ph}.

- The wave packet now can be written with new form as:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{ik_o(x-v_{ph}t)} \int_{-\infty}^{+\infty} g(k - k_o)\, e^{i(k-k_o)(x-v_g t)} e^{-i(k-k_o)^2\alpha t + \cdots}\, \mathrm{dk};$$

Where $v_g = \frac{d\omega(k)}{dk}$ is group velocity and $v_{ph} = \frac{\omega(k)}{k}$ is phase velocity

- The phase velocity denotes the velocity of propagation for the phase of a single harmonic wave, $e^{ik_o(x-v_{ph}t)}$, and the group velocity represent s the velocity of motion for the group of waves that make up the packet.

iv. Group and phase velocity

- When we superimpose many waves of different amplitudes and frequencies. We can obtain a wave packet or pulse which travels at the group velocity v_g: the *individual* wave that constitute the packet.
- However, this wave packet moves with different speeds; each wave moves with its own phase velocity v_{ph}.
- The group velocity represents the velocity with which the wave packet propagates as a *whole*, where the individual waves (located inside the packet's envelope) that add to make the packet move with different velocities.
- The difference between the group velocity and the phase velocity can be understood quantitively by deriving the relation between them.
- As aforementioned in the previous paragraph, the phase velocity defined as

$$v_{ph} = \frac{\omega(k)}{k}$$

From this equation, we can define ω as a function to k with proportional constant v_{ph} :

$\omega = kv_{ph}$, and its derivative to k is $v_g = \frac{d\omega}{dk} = v_{ph} + k\left(\frac{dv_{ph}}{dk}\right)$,

And since $k = \frac{2\pi}{\lambda}$, we have $\left(\frac{dv_{ph}}{d\lambda}\right)\left(\frac{d\lambda}{dk}\right) = -\left(\frac{2\pi}{k^2}\right)\left(\frac{dv_{ph}}{d\lambda}\right)$ or $k\left(\frac{dv_{ph}}{dk}\right) = -\lambda\left(\frac{dv_{ph}}{d\lambda}\right)$,

Therefore, v_g can be write as equation follows:

$$v_g = \frac{d\omega}{dk} = v_{ph} + k\left(\frac{dv_{ph}}{dk}\right) = v_{ph} - \lambda\left(\frac{dv_{ph}}{d\lambda}\right)$$

Which can also write as

$$v_g = v_{ph} + p\left(\frac{dv_{ph}}{dp}\right)$$

Since $k\left(\frac{dv_{ph}}{dk}\right) = \left(\frac{p}{\hbar}\right)\left(\frac{dv_{ph}}{dp}\right)\left(\frac{dv_p}{dk}\right) = p\left(\frac{dv_{ph}}{dp}\right)$ because $k = \frac{p}{\hbar}$.

- It is clear from equations above; the group velocity may be larger or smaller than the phase velocity; it may be equal to the phase velocity depending on the medium.
- If the phase velocity does not depend on the wavelength-this occurs in nondispersive media- the group and phase velocities are equal, since $\frac{dv_{ph}}{d\lambda} = 0$.
- But if v_{ph} depends on the wavelength-this occurs in dispersive media- then $\frac{dv_{ph}}{d\lambda} \neq 0$, hence the group velocity may be smaller or larger than the phase velocity.

Exercises:

Q.1:

(a) Find the Fourier transform for $\emptyset(k) = \begin{cases} A(a - |k|), & |k| \leq a \\ 0, & |k| > a \end{cases}$, where is positive parameter and A is normalization factor to be found.

(b) Calculate the uncertainties Δx and Δp, and check whether satisfy the uncertainty principle.

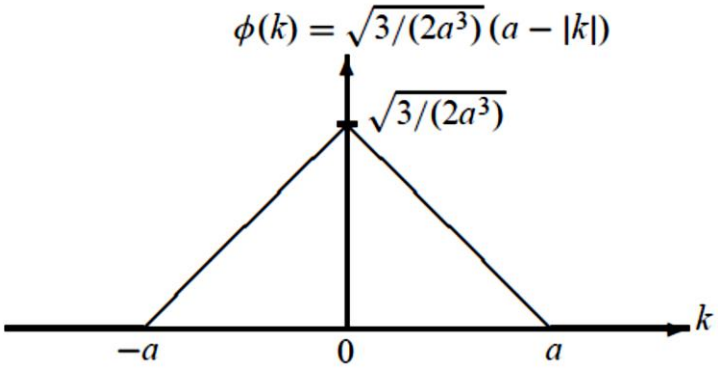
Solution:

(a) The normalization factor can be found at once:

$$1 = \int_{-\infty}^{+\infty} |\emptyset(k)|^2 dk = |A|^2 \int_{-a}^{0} (a+k)^2 dk + |A|^2 \int_{0}^{a} (a-k)^2 dk$$
$$= 2|A|^2 \int_0^a (a-k)^2 dk = 2|A|^2 \int_{-0}^{a} a^2 - 2ak + k^2 dk$$
$$= \frac{2a^3}{3}|A|^2,$$

Then $A = \sqrt{3/(2a^3)}$.

The shape of $\phi(k) = \sqrt{3/(2a^3)}\,(a - |k|)$, is display in Figure below.



Now, the Fourier transform of $\phi(k)$ is

$$\psi_o(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \emptyset(k)\, e^{ikx} dk$$

$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{3}{2a^2}} \left[\int_{-a}^{0} (a+k) e^{ikx}\, dk + \int_{0}^{a} (a+k) e^{ikx}\, dk \right]$$

$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{3}{2a^2}} \left[\int_{-a}^{0} k e^{ikx}\, dk - \int_{0}^{a} k e^{ikx}\, dk + a \int_{-a}^{a} e^{ikx}\, dk \right]$$

Using the integrations

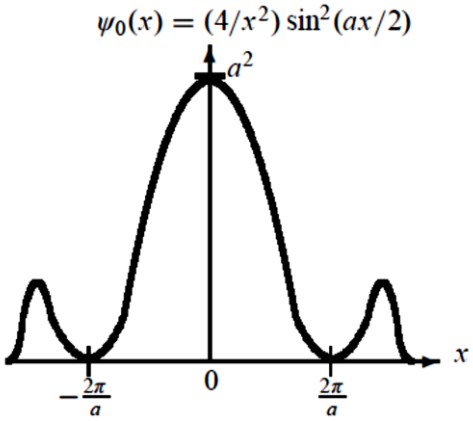
$$\int_{-a}^{0} k e^{ikx}\, dk = \frac{a}{ix} e^{-iax} + \frac{1}{x^2}\left(1 - e^{-iax}\right),$$
$$\int_{0}^{a} k e^{ikx}\, dk = \frac{a}{ix} e^{iax} + \frac{1}{x^2}\left(e^{iax} - 1\right),$$
$$\int_{-a}^{a} e^{ikx}\, dk = \frac{1}{ix}\left(e^{iax} - e^{-iax}\right) = \frac{2sin(ax)}{x},$$

And after some straightforward calculations, we end up with

$$\psi_o(x) = \frac{4}{x^2} sin^2\left(\frac{ax}{2}\right)$$

As shown in Figure below, this wave packet is localized it peaks at $x = 0$ and decrease gradually as x increase. We can verify that maximum of $\psi_o(x)$ ocuurs

at $x = 0$, writing $\psi_o(x)$ as $a^2(ax/2)^{-2}sin^2(ax/2)$ and since $\lim x \to 0\ sin(bx)/(bx) \to 1$, we obtain $\psi_o(0) = a^2$.



(b) Figure of $\phi(k)$ is quite suggestive indefining the half width $\phi(k)$: $\Delta k = a$ (hence the momentum uncertainty is $\Delta p = \hbar a$). By defining the width as $\Delta k = a$, we known with full certainty that the particle is located between $-a \leq k \leq a$; according to Figure of $\phi(k)$, the probability of finding the particle outside the interval is zero, for $\phi(k)$ vanishes when $|k| > a$.

Now, let us find the width Δx of $\psi_o(x)$. Since $sin(a\pi/2a) = 1$, $\psi_o(\pi/a) = 4a^2/\pi^2$, and that $\psi_o(0) = a^2$, we can obtain from $\psi_o(x)$ that $\psi_o(\pi/a) = 4a^2/\pi^2 = 4/\pi^2\ \psi_o(0)$ or

$$\frac{\psi_o(\pi/a)}{\psi_o(0)} = \frac{4}{\pi^2}$$

This suggest that $\Delta x = \pi/a$,when $x = \mp\Delta x = \mp\pi/a$ the wave packet $\psi_o(x)$ drops to $4/\pi^2$ from its maximum value $\psi_o(x) = a^2$. In sum, we have $\Delta x = \pi/a$ and $\Delta k = a$, hence

$$\Delta x \Delta k = \pi \quad \text{or} \quad \Delta x \Delta p = \pi\hbar$$

Since $\Delta k = \Delta p/\hbar$. In addition to satisfying Heisenberg's uncertainty principle, this relation shows that the product $\Delta x \Delta p$ is higher than $\hbar/2$: $\Delta x \Delta p > \hbar/2$ .The wave packet $\psi_o(x)$ therfore offers a clear illustration of the general statement outlined above, namely, only Gaussian wave packets yields the *lowest* limit to Heisenberg's uncertainty principle $\Delta x \Delta p > \hbar/2$, All other wave packets , yields higher value for the product $\Delta x \Delta p$.

Q.2. Calculate the group and phase velocities for the wave packet corresponding to a relativistic particle.

Solution:

Recall that the energy and momentum of a relativistic particle is given by

$$E = mc^2 = \frac{m_o c^2}{\sqrt{1 - v^2/c^2}}, \quad p = mv = \frac{m_o v}{\sqrt{1 - v^2/c^2}}$$

Where m_o is the rest mass of the particle and c is the speed of light in a vaccum.

Squaring and adding the expressions of E and p, we obtain $E^2 = p^2c^2 + m_o^2c^4$; hence

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

Using the relation along with $p^2 + m_o^2c^2 = m_o^2c^2/(1 - v^2/c^2)$ and $v_g = dE(p)/dp$, $v_{ph} = E(p)/p$, we can show that the group velocity is given as follow:

$$v_g = \frac{dE(p)}{dp} = \frac{d}{dp}\left(c\sqrt{p^2 + m_o^2c^2}\right) = \frac{pc}{\sqrt{p^2 + m_o^2c^2}} = v$$

The group velocity is thus equal to the speed of the particle $v_g = v$.

The phase velocity can be found from $v_{ph} = E/p$ and $E = c\sqrt{p^2 + m_o^2c^2}$:$v_{ph} = E/p = c\sqrt{1 + m_o^2c^2/p^2}$ which combined with $p = m_o v/\sqrt{1 - v^2/c^2}$, leads to $\sqrt{1 + m_o^2c^2/p^2} = c/v$; hence

$$v_{ph} = \frac{E}{p} = c\sqrt{1 + \frac{m_o^2c^2}{p^2}} = \frac{c^2}{v}$$

This show that the phase velocity pf the wave corresponding to a relativistic particle with m_o is larger than the speed of light, $v_{ph} = c^2/v > c$. *This indeed unphysical*. The result $v_{ph} > c$ seems to violate the special theory of relativity, which state that the speed of material particles cannot exceeds c. In fact, this principle is not violated because v_{ph} does not represent the velocity of particle: the velocity of particle is represented by the group velocity. As a result, the phase speed of a relativistic particle has no meaningful physical significance.

Finally, the product of the group and phase velocities is equal to c^2 i.e., $v_g v_{ph} = c^2$.

Q.3. The angular frequency of the surface waves in a liquid is given in terms of the wave number k by $w = \sqrt{gk + Tk^3/\rho}$, where g is the accelaration due to gravity, ρ is the density of the liquid,and T is the surface tension(which gives an force on an element of the surface liquid). Find the phase and group velocities for the limiting cases when surface waves have: (a) very large wavelengths and (b) very small wavelengths.

Solution.

The phase velocity can be found at once from equation following:

$$v_{ph} = \frac{w}{k} = \sqrt{\frac{g}{k} + \frac{T}{\rho}k} = \sqrt{\frac{g\lambda}{2\pi} + \frac{2\pi T}{\rho\lambda}}$$

Where we have used the fact that $k = 2\pi/\lambda$, λ being the wavelength of the surface waves.

(a) If λ is very large, we can neglect the second term in eq. above; hence

$$v_{ph} = \sqrt{\frac{g\lambda}{2\pi}} = \sqrt{\frac{g}{k}}$$

In this approximation the phase velocity does not depend on the nature of the liquid,

since it depends on no parameter pertaining to the liquid such as its density or surface tension. This case corresponds, for instance, to deep-water waves, called gravity waves.

To obtain the group velocity,

let us differentiate v_{ph} with respect to k: $dv_{ph}/dk = -(1/2)\sqrt{g/k} = -v_{ph}/2k$.

A substitution of this relation into v_g shows that the group velocity is half the phase velocity:

$$v_g = \frac{dw}{dk} = v_{ph} + k\frac{dv_{ph}}{dk} = v_{ph} - \frac{1}{2}v_{ph} = \frac{1}{2}v_{ph} = \frac{1}{2}\sqrt{\frac{g\lambda}{2\pi}}$$

The longer the wavelength, the faster group velocity. This explains why a strong, steady wind will produce waves of longer wavelength than those produced by a swift wind.

(b) If is very small, the second term in v_{ph} becomes the dominate one. So, retaining only the second term, we have

$$v_{ph} = \sqrt{\frac{2\pi T}{\rho\lambda}} = \sqrt{\frac{T}{\rho}k}$$

Which leads to $dv_{ph}/dk = \sqrt{Tk/\rho}/2k$. inserting this expression into v_g, we obtain the group velocity

$$v_g = v_{ph} + k\frac{dv_{ph}}{dk} = v_{ph} + \frac{1}{2}v_{ph} = \frac{3}{2}v_{ph}$$

Hence the smaller the wavelength, the faster the group velocity. These are called ripple waves; they occur, for instance, when a container is subject to vibrations of high frequency and small amplitude or when a gentle wind blows on the surface of a fluid.