



Engineering Physics

(PHY1701)

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- **Wave function (AB 182-184 & 190-195), &**
- Schrödinger equation (time dependent & independent) (AB 187 -190 & 195-197).

❖ Concepts of Modern Physics, Arthur Beiser et al., Sixth Edition, Tata McGraw Hill (2013) (AB)

Heisenberg Uncertainty Principle

❖ History:

In 1927, the German physicist '**Werner Heisenberg**' developed the uncertainty principle.



Werner Heisenberg

Uncertainty Principle

- ✓ Quantum mechanics predicts that a barrier to measurements with ultimately small uncertainties does exist.

❖ Statement:

"It is **impossible to accurately determines** both the **position** and **momentum** of **any particles simultaneously**."

- This is not due to the instrumental limitation.
- This limitation exist in nature itself.
- If a measurement of position of a particle is made with precision Δx and a simultaneous measurement of linear momentum is made with precision Δp , then the product of the two uncertainties can never be smaller than $h/4\pi$.

uncertainty in momentum

↓

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

↑

uncertainty in position

❖ Uncertainty Principle :

Our microscope thought experiments give us a rough estimate for the uncertainties in position (x) and momentum (p):

$$\Delta x \Delta p \sim h$$

Here, Δx : Change/uncertainty of position,
 Δp : Change/uncertainty of momentum,
 h : Plank's constant ($6.62607015 \times 10^{-34}$ J.s)

“Formal” statement of the Heisenberg uncertainty principle:

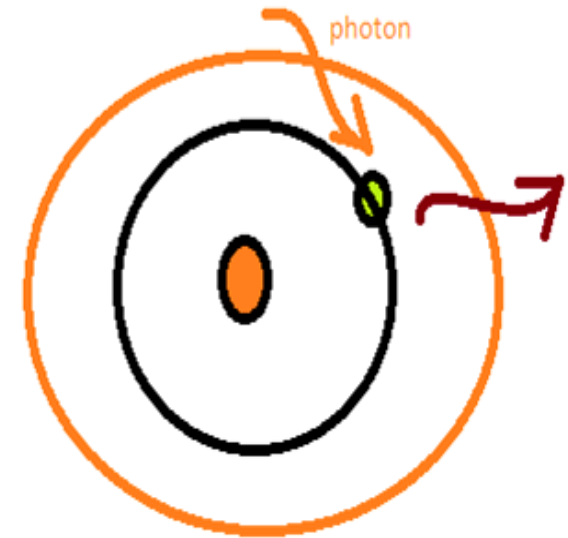
$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

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

$$\text{Since, } \hbar = \frac{h}{2\pi}$$

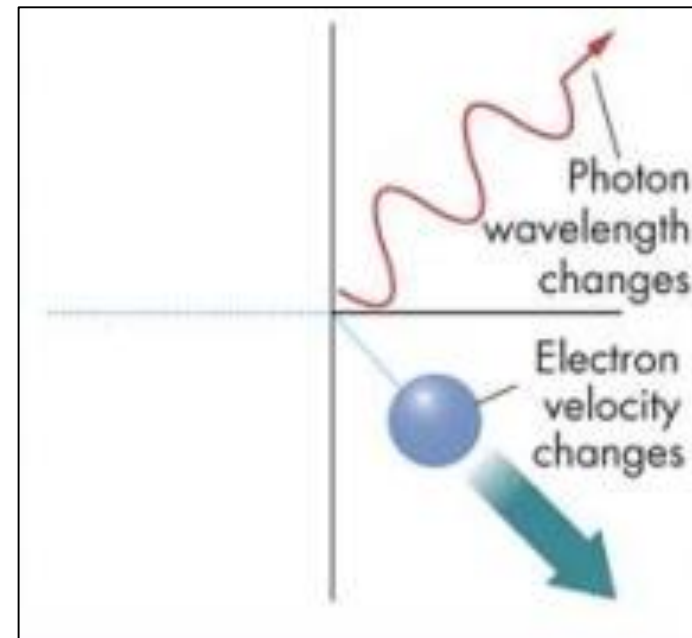
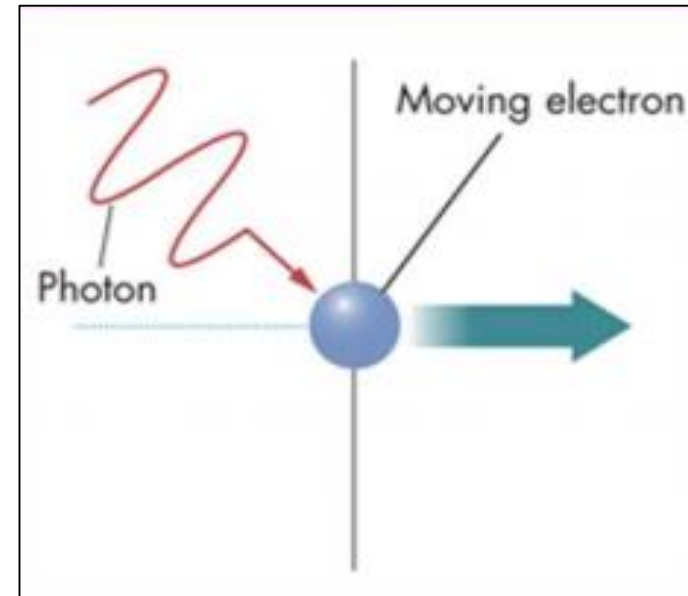
Heisenberg Experiment to measure Uncertainty

- Heisenberg made an experiment that, he took high **electromagnetic radiation** and made passed through the electron which is revolving around the nucleus.
- Electromagnetic radiation hits the electron, we can measure the position of electron, there may an other possibilities that electron must deviate from that orbital.
- Hence, we can't determine the momentum simultaneously.
- According to de-Broglie equation the mass is **inversely proportional** to wavelength.
- From that equation the **wavelength** electromagnetic radiation should be higher than the **mass of the electron**.
- According to this principle the position and momentum of a particle (say electron) cannot be determined simultaneously to any desired degree of accuracy.



Measuring the p and x of electron:

- ✓ To determine the position accurately it is necessary to use light with a short wavelength
- ✓ By Planck's law $E = hc/\lambda$, a photon with a short wavelength has a large energy. So will give a large 'kick' to the electron
- ✓ But to determine its momentum accurately, electron must only be given a small kick
- ✓ This means using light of long Wavelength
- ✓ Although experiment for viewing an electron is with a powerful microscope.
- ✓ In order to see the electron, at least one photon must bounce off it.
- ✓ During this interaction, momentum is transferred from the photon to the electron.
- ✓ Therefore, the light that allows you to accurately locate the electron changes the momentum of the electron.
- ✓ The change in the momentum of electron is $\Delta p \approx \frac{h}{\lambda}$



Heisenberg Uncertainty Principle

- If we choose a photon with larger wavelength, then the position error will be equivalent to the wavelength of the photon, since the electron can be situated anywhere within the wavelength of the photon.

$$\Delta x \approx \lambda$$

- There can be

$x_1, x_2, x_3 \dots x_n$ possible position values within Δx position range
and

$p_1, p_2, p_3 \dots p_n$ possible momentum values within Δp momentum range

- For any position value, among $x_1, x_2, x_3 \dots x_n$,
the possible **momentum** values are in Δp momentum range
- Similarly, for any momentum value, among $p_1, p_2, p_3 \dots p_n$
the possible **position** values are Δx position range

Heisenberg Uncertainty Principle

- Therefore, the total minimum uncertainty is

$$\Delta x \cdot \Delta p \approx \lambda \cdot \frac{h}{\lambda} \approx h$$

the uncertainty will be $\Delta x \cdot \Delta p \geq h$

$$\frac{\Delta x}{\Delta t} = v \rightarrow \Delta x = v \Delta t$$

$$E = \frac{p^2}{2m}; \quad \Delta E = \frac{2p\Delta p}{2m} \rightarrow \Delta E = \frac{mv\Delta p}{m} \rightarrow \Delta p = \frac{\Delta E}{v}$$

$$v\Delta t \cdot \frac{\Delta E}{v} = \Delta E \cdot \Delta t \geq h$$

- ❖ The final minimum uncertainties are:

$$\Delta x \cdot \Delta p \geq h$$

$$\Delta E \cdot \Delta t \geq h$$

- ❖ The final accurate uncertainties are:

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

$$\Delta E \Delta t \geq \frac{h}{4\pi}$$

Applications of Uncertainty Principle

- ✓ Non-existence of electron in the nucleus
- ✓ Zero- point energy of a harmonic oscillator
- ✓ Ground state energy and the radius of the hydrogen atom
- ✓ Evidence for finite width of the spectral lines
- ✓ Binding energy of an electron in atom

WAVE FUNCTION

- In 1926, **Erwin Schrödinger** proposed a wave equation that describes the manner in which matter waves change in space and time.
- It is denoted by the greek word Ψ . In general wave function represented by $\Psi(\mathbf{r},t)$ where \mathbf{r} -space, t - time



- The wave function depends on the particle's position and the time
- Schrödinger's wave equation is a key element in quantum mechanics:

$$i \frac{\Delta \Psi}{\Delta t} = H \Psi$$

- Schrödinger's wave equation is generally solved for the wave function, " Ψ ".

Wave Function

- In quantum mechanics the object is described by a **state** (not trajectory).
- The state is characterized by a complex **wave function Ψ** , which depends on particle's position and the time.
- The wave function is interpreted as a **probability amplitude** of particle's presence.
- The **probability density** (probability of finding the object at time t inside an elementary volume $dx dy dz$):

$$|\Psi(x, y, z, t)|^2 dx dy dz$$

➤ Let us first consider 1D systems.

➤ Then, the probability of finding a particle between a and b, at time t:

$$\int_a^b |\Psi(x, t)|^2 dx$$

➤ Since the particle should be somewhere:

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

➤ This is called **normalization** condition.

Physical Significance of ψ :

- ✓ By applying Schrödinger equation to the motion of a particle, we get the wave function Ψ .
 - ✓ The quantity whose variation make up **matter wave** is called the wave function Ψ . This function can be either **real or complex**.
 - ✓ The wave function ψ itself, has **no direct physical** significance.
 - ✓ The only quantity having a physical meaning is the square of its magnitude **$P = |\Psi|^2 = \Psi^*$** . Here, Ψ^* is the complex conjugate of Ψ .
- OR*
- ✓ $|\Psi|^2$ the square of the absolute value of the wave function, is called **probability density**.

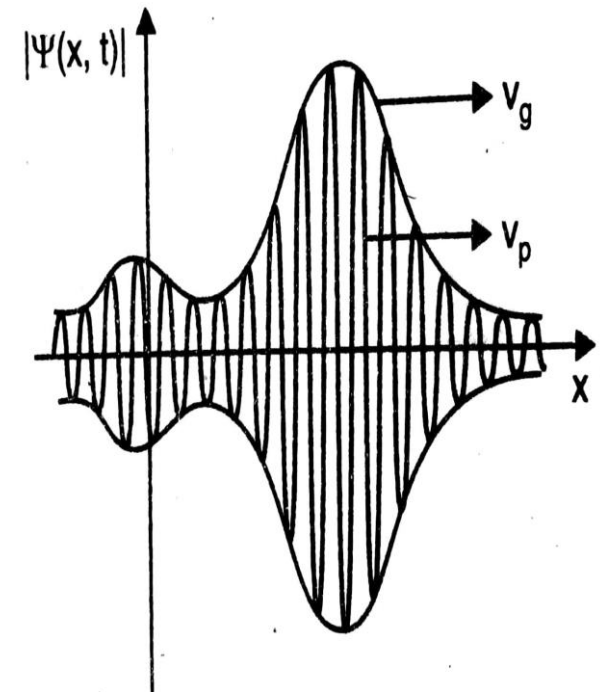
Properties of Wave Function

- ✓ Ψ defines the dynamical state of a system.
- ✓ Ψ is a complex quantity
- ✓ Ψ must be finite for all values of x, y, z .
- ✓ Ψ must be single valued
- ✓ Ψ must be continuous in all regions except where the potential energy is infinite.
- ✓ Ψ must possess continuous first order derivative everywhere
- ✓ Ψ vanishes at the boundaries.
- ✓ Every wave function must satisfy normalization condition. $\iiint_{-\infty}^{\infty} |\psi|^2 dx dy dz = 1$
- ✓ A wave function satisfying the following condition is called orthogonal wave function.

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 0$$

Wave Packet

- A particle in motion is represented by a wave that is confined to **a small region of space** around the particle, such wave is called **Wave packet**.
- A wave packet is the superposition of a large number of waves.
- The wave interfere **constructively** in the vicinity of the particle, giving the resultant wave a large amplitude.
- The wave interfere **destructively** far from the particle.
- So the wave has small amplitude in region.
- The figure shows a wave packet propagating along the X-axis.
- It consists of “**ripples**” contained within an “**envelope**”.
- The “envelope” travels at the **group velocity (v_g)**.
- The individual ripples travel at the **phase velocity (v_p)**.



Operators

- An operator is one which tells what operation to carryout on the quantity that follows it.
- Let us consider the free particle wave function:
- Differentiating w.r.t. x and t, we get:

$$\Psi = Ae^{-\left(\frac{i}{\hbar}\right)(Et - px)}$$

$$\frac{\partial \Psi}{\partial x} = \frac{i}{\hbar} p \Psi \quad \frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} E \Psi$$

- Rewriting we get,

$$p \Psi = -i\hbar \frac{\partial \Psi}{\partial x} \quad E \Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

- Here, $p \Psi = -i\hbar \frac{\partial \Psi}{\partial x}$ is defined as **Momentum Operator** and

$$E \Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad \text{is defined as } \mathbf{Energy Operator}.$$

Identifying the operators

$f(x)$	Any function of position, such as x , or potential $V(x)$	$f(x)$
p_x	x component of momentum (y and z same form)	$\frac{\hbar}{i} \frac{\partial}{\partial x}$
E	Hamiltonian (time independent)	$\frac{p_{op}^2}{2m} + V(x)$
E	Hamiltonian (time dependent)	$i\hbar \frac{\partial}{\partial t}$
KE	Kinetic energy	$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
L_z	z component of angular momentum	$-i\hbar \frac{\partial}{\partial \phi}$

Eigen Value

- In any measurement of the observable associated with the **operator** \hat{G} , the only values that will ever be observed are the **Eigen values** “ G_n ”, which satisfy the Eigen value equation:

$$\hat{G}\Psi_n = G_n\Psi_n$$

- This is the postulate that the values of dynamical variables are quantized in quantum mechanics.
- **Eigen Function and Eigen values:**

$$\hat{G}f(x) = kf(x)$$

Here, $f(x)$ is eigen function of \hat{G} with eigen value k

Eigen Value

- If an operator (\hat{G}), acting on a wave function Ψ_n such that

$$\hat{G}\Psi_n = G_n\Psi_n$$

- Then G_n is called as Eigen value of the given function.

-
- For Example, let $\Psi = e^{2x}$ and $\hat{G} = \frac{d^2}{dx^2}$

- Now $\hat{G}\Psi = \frac{d^2}{dx^2}(e^{2x}) = 4e^{2x} = 4\Psi$

- Here **4 is the Eigen value** for the **function of e^{2x}** with operator $\frac{d^2}{dx^2}$

Eigen values

- All observable values ω_n , for a system in state Ψ_n obey the eigenfunction-eigenvalue relationship. The subscript n indicates a whole family of solutions, with each member given by a quantum number n .

$$\hat{Q} \psi_n = \omega_n \psi_n$$

eigenvalue equation

(operator)(function) = (constant factor) × (function)

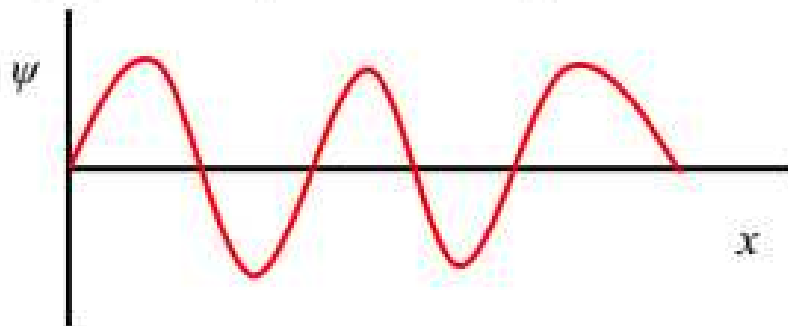
↖ ↗
eigenfunction,
eigenstate or
eigenvector

eigenvalue

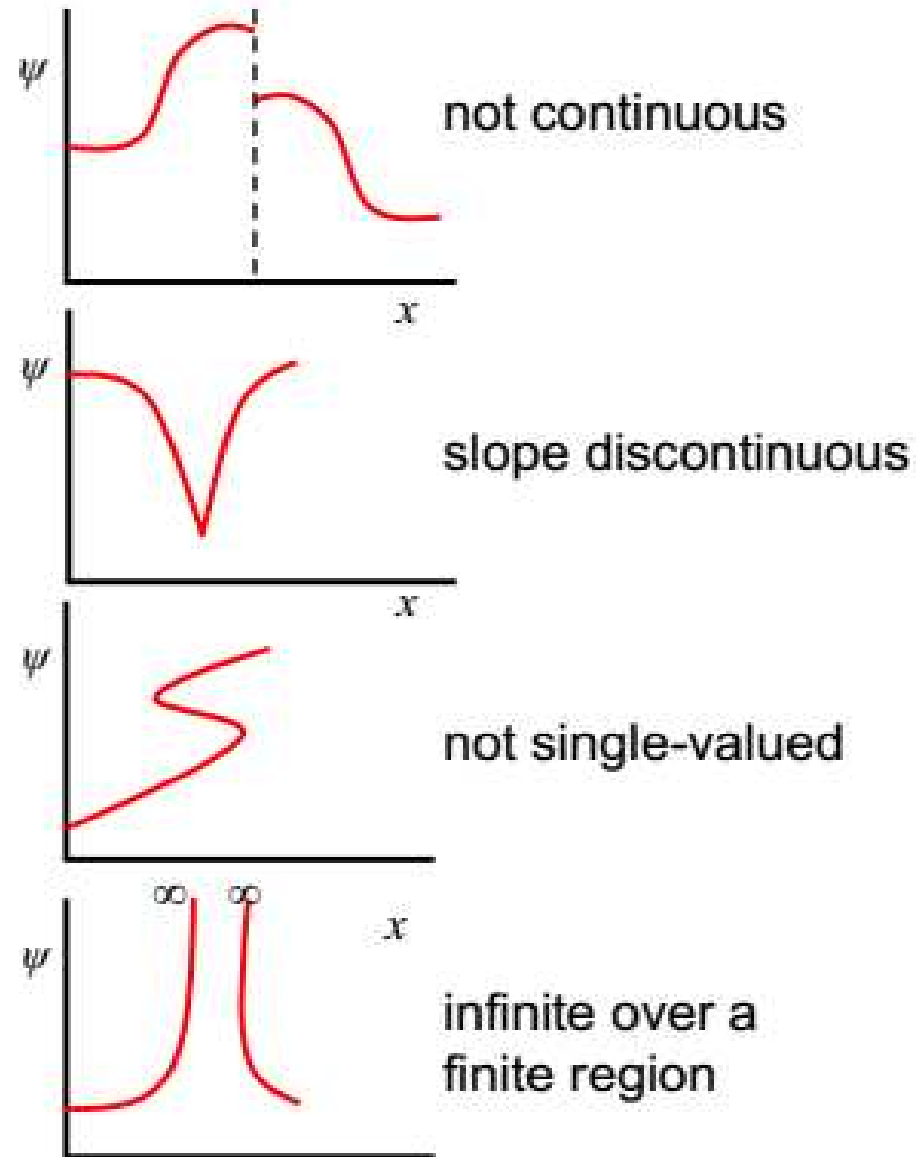
Acceptable wave function

An acceptable wavefunction must:

- (i) be continuous,
- (ii) have a continuous slope,
- (iii) be single-valued,
- (iv) be square-integrable.



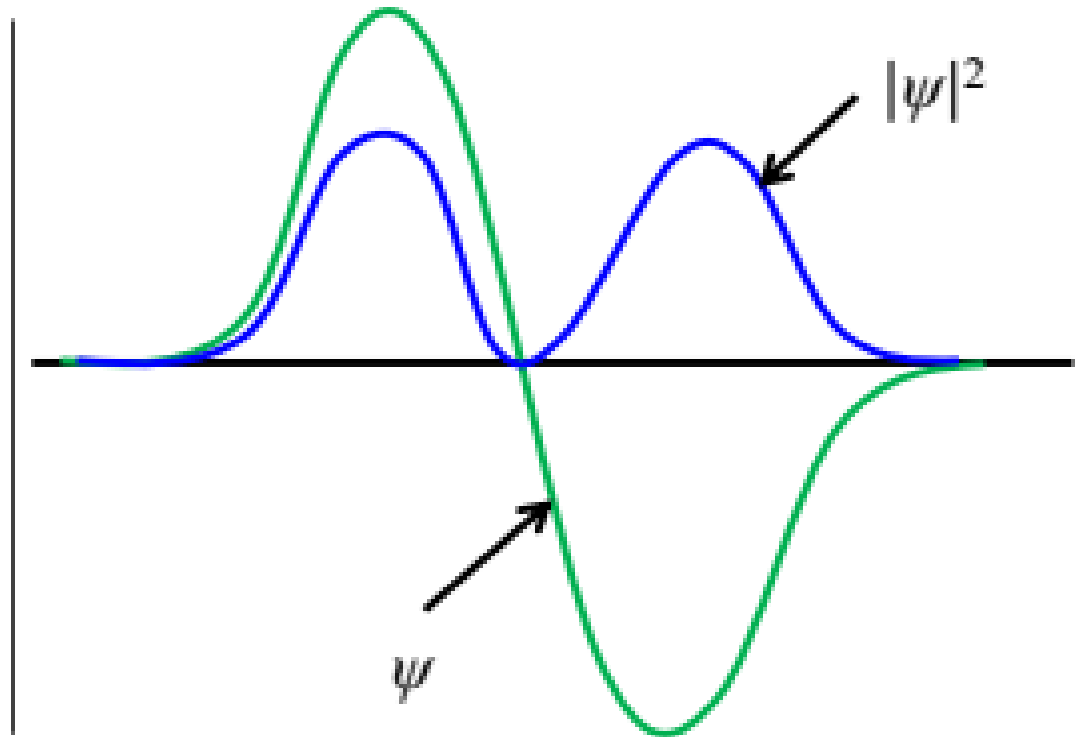
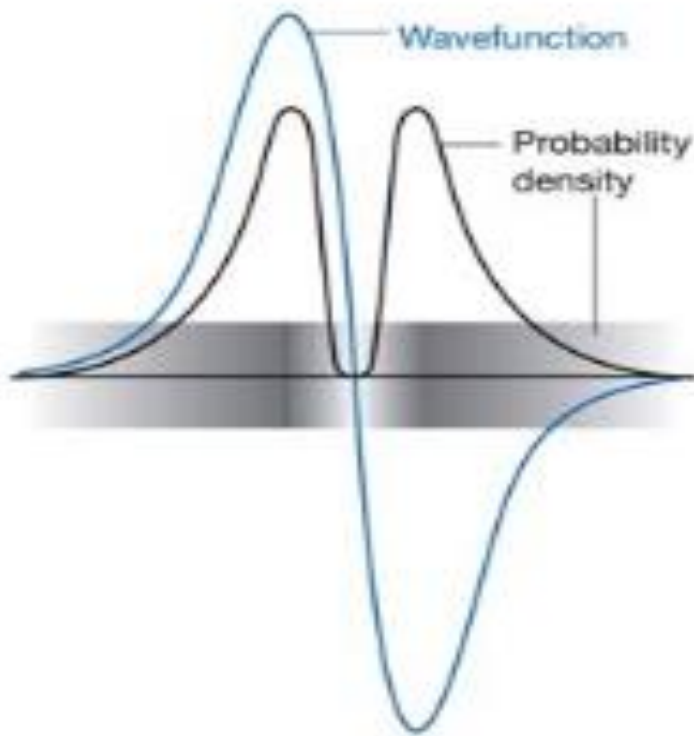
An acceptable wavefunction, e.g. functions of \sin and \cos .



Unacceptable wavefunction, e.g. functions of \tan

Wave function and probability density

- The sign of a wave function has no direct physical significance
- The positive and negative regions of this wave function both correspond to the same probability distribution.



Law of Equipartition of Energy

➤ For a system in thermal equilibrium, the law of Equipartition of Energy states that the total energy for the system is equally divided among the degree of freedom.

➤ According to the kinetic theory of gases, the average kinetic energy of molecule is given by,

$$\frac{1}{2}mv_{rms}^2 = \frac{3}{2}k_bT$$

, where V_{rms} is the root mean square velocity of the molecules, K_b is the Boltzmann constant and T is the temperature of the gas.

➤ The mono-atomic gas has three degree of freedom, so the average kinetic energy per degree of freedom is given by

$$KE_x = \frac{1}{2}k_bT$$

$$\frac{1}{2}kT$$

per molecule

$$\frac{1}{2}RT$$

per mole

k = Boltzmann's constant

R = gas constant

$$\frac{3}{2}kT$$

$$\frac{3}{2}RT$$

For three translational degrees of freedom, such as in an ideal monoatomic gas,

Position	$r(x, y, z)$	Multiply by $r(x, y, z)$
Momentum	$p(p_x, p_y, p_z)$	$-i\hbar \nabla$
Kinetic energy	$T = \frac{p^2}{2m}$	$-\frac{\hbar^2}{2m} \Delta$
Potential energy	$\Phi(r)$	Multiply by $\Phi(r)$
Total energy	$E = T + \Phi$	$i\hbar \frac{\partial}{\partial t} = \Phi(r) - \frac{\hbar^2}{2m} \Delta$
Angular momentum	(l_x, l_y, l_z)	$-i\hbar \mathbf{r} \times \nabla$

Observable	Classical Symbol	Quantum Operator	Operation
position	\mathbf{r}	$\hat{\mathbf{r}}$	multiply by \mathbf{r}
momentum	\mathbf{p}	$\hat{\mathbf{p}}$	$-i\hbar(\hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z})$
kinetic energy	T	\hat{T}	$\frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$
potential energy	$V(\mathbf{r})$	$\hat{V}(\mathbf{r})$	multiply by $V(\mathbf{r})$
total energy	E	\mathcal{H}	$\frac{-\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}) + V(\mathbf{r})$
angular momentum	l_x	\hat{l}_x	$-i\hbar(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y})$
	l_y	\hat{l}_y	$-i\hbar(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})$
	l_z	\hat{l}_z	$-i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$