# Fundamental wave-particle relations:

$\lambda$: wavelength

Frequency: $f = \frac{E}{h}$ $\qquad \hbar = h/2\pi$

wave number: $k = \frac{2\pi}{\lambda}$

angular frequency: $\omega = \frac{2\pi}{T}$

De Broglie

$$p = \frac{h}{\lambda} = h \cdot 2\pi k = \hbar k$$

$$E = hf = \hbar \omega$$

FUNDAMENTAL WAVE PARTICLE RELATIONSHIPS

For each wave, there is a wave equation of which the w.f. is a solution

{ ex. electromagnetic wave, follow Maxwell equation }

$\nabla \cdot E = 0$ , $\nabla \times E = -\frac{\partial B}{\partial t}$ ; $\nabla \cdot B = 0$ ; $\nabla \times B = \mu_0 \varepsilon_0 \frac{\partial E}{\partial t}$

classical wave eq. $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$

Matter waves follow the Schrödinger equation:

- we consider a free particle (no external forces):

Eq:
$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

Meaning Born's statistical interpretation:

$|\psi(x,t)|^2 dx$ : probab. of finding a particle between $x, x+dx$ at time $t$

- **FREE PARTICLE :**

we guess a possible solution:

PLANE WAVE $\psi(x,t) = A e^{i(Kx - wt)}$

is it a sol?

$$+\frac{\hbar^2}{2m}K^2\left[A e^{i(Kx-wt)}\right] = \hbar w A e^{i(Kx-wt)}$$

$$\rightarrow \frac{\hbar^2 K^2}{2m} = \hbar w \rightarrow \frac{p^2}{2m} = E$$

{ wave eq. $f$: $x \pm vt$
$e^{ik(x - w/k\, t)}$ ; this is a wave with $v = \frac{w}{k} = \sqrt{\frac{E}{2m}}$ }

It is telling us that for a free particle,

KIN. ENERGY = TOTAL ENERGY

the schr. eq. is related to a classical accounting of ENERGY

The square of the wave function absolute value gives: probability/[unit of length] of finding the particle: $|\psi(x,t)|^2$

SUMMARY

- FREE PARTICLE SCHRÖDINGER EQUATION:

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

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

$$\frac{\hbar^2 k^2}{2m} = \hbar\omega$$

- FUNDAMENTAL PARTICLE-WAVE EQS

$$p = \frac{\pi}{\lambda} = \hbar k$$

$$E = h\nu = \hbar\omega$$

$$\psi(x,t) = A\,e^{\frac{i}{\hbar}(px-Et)}$$

# PHYSICAL CONDITIONS: WELL BEHAVED WAVE FUNCTIONS

The probability of finding a particle between $x - x+dx$: $P(x)\,dx = \psi^*(x,t)\psi(x,t).dx$

PROBABILITY DENSITY

The probability of observing it between $x_1$ and $x_2$ is:

$$P = \int_{x_1}^{x_2} \psi^* \psi \, .dx$$

- The particle must exist somewhere → this condition is imposed NORMALIZING the w.f [the extreme of integr. are $\mp\infty$]

$$\int_{-\infty}^{\infty} \psi(x,t)^* \psi(x,t) = 1$$

to be physically acceptable a w.f. must be normalizable

e.g. to represent a particle

P.W. $\int_{-\infty}^{\infty} dx\, |A|^2 . e^{i(kx-wt)} . e^{-i(kx-wt)} = \infty$

* important property of schr. eq. is that it preserves the normaliz. at all times [ Griffith eq. 1.21 and following ]

→ we can undestand it using the uncertainty principle. The problem with this wave is that cannot represent a particle whose w.f. is nonzero in a limited region of space. A localized wavefunction of this type is called $\underbrace{\text{wave packet}}$

- SMOOTHNESS: w.f. smooth, 1 deriv. smooth, if not the K.E. could be $\infty$

## What are expectation values:

For a particle in a state $\Psi$, the expectation value of $x$ is:

$$\langle x \rangle = \int dx\, x\, \Psi^*(x)\Psi(x)$$

- what does it mean? It does not mean that if you measure the position of a particle over and over $\int x\, dx |\Psi|^2$ is the average of the results that you obtain

$\langle x \rangle$ is the average of measurements performed on particles ALL in state $\Psi$. Which means: - you prepare a whole ensamble of particles each in the same state $\Psi$ and measure the positions of all of them $\langle x \rangle$ is then the average of these results

The expectation value is the average of repeated measurements on an ensamble of identically prepared systems; NOT the average of repeated measurements on the same system.

- we say the operator $\hat{x}$ "represents" position; to calculate its expectation value we sandwich the appropriate operator between $\Psi$ and $\Psi^*$ & integrate

$$\langle Q \rangle = \int dx\, \Psi^*\, Q\, \Psi$$

OPERATOR: is an instruction to do something on the function that follows it; the position operator tells you to multiply by '$x$'
the mom. oper. tells you to differentiate w respect to $x$.

## Well Defined Observables: Eigenvalues

Given an operator $\hat{Q}$, the function $f(x)$ is an eigenfunction of the operator, if and only if the operator acting on the function yields a constant times the same function:

$$\hat{Q}\, \underbrace{f(x)}_{\text{eigenfunction}} = \underbrace{\lambda}_{\text{Eigenvalue}}\, f(x)$$

In general, an operator will have multiple eigenvalues

### EIGENVALUES, EIGENVECTORS

* How does it work for matrices?

We say $v$ is an eigenvector of $M$ if: $Mv = \underbrace{c}_{\text{is a number, eigenvalue}} v$

Example: $\boxed{\text{POLL}}$

$$\begin{bmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{bmatrix} \rightarrow \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

What are the eigen values:

$1, 1, 1$ (A)

$0, 0, 0$ (B)

$a_1, a_2, a_3$ (C)

## Heisenberg Uncertainty Relation:

The mere fact that a phenomenon has a wave nature implies inherent uncertainty in its particle properties.

What do we mean by "uncertanty" in an observable?

That if we measure many times the same obs., the number I find varies in a range of values

UNCERTAINTY ⟶ MEASURE HOW FAR DEVIATIONS ARE FROM THE MEAN AVERAGE VALUE

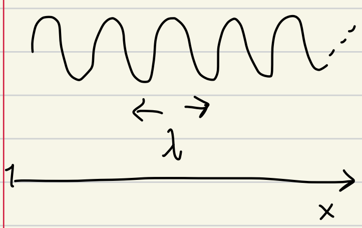
## HEISENBERG UNCERTAINTY PRINCIPLE:

→ Because of a particle wave's nature, it is theoretically impossible to know precisely both its position along an axis and its momentum component along that axis

- $\Delta x$ and $\Delta p_x$ cannot be zero simultaneously

$$\Delta p_x \cdot \Delta x \geq \frac{\hbar}{2}$$ (Heisenberg Nobel prize 1932)

Examples to better understand the uncertainty principles:




this wave if infinite and regular

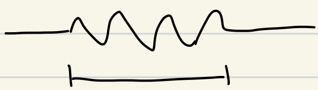
well defined wavelength $\lambda$

$p = \frac{h}{\lambda}$ ; Any idea on $\Delta p$?

$\Delta P_x$ is 0; but we don't know anything about its position

$\Delta x = \infty$

Wave is regular over a finite region
Not everywhere $\left\{ \lambda \text{ and } p \text{ not well defined} \right\}$

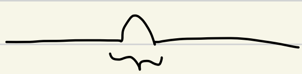


$\Delta x$ is finite

$\Delta p \neq 0$

Better known position.

we further restricted the region where the wave is regular and we can define $\lambda, p$



$\Delta x$ is small

## HAMILTONIAN:

In classical mechanics the total energy:
kin + potential is called: Hamiltonian

Hamiltonian = kin. en + pot. en

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

the Hamiltonian operator obtained by the canonical substit.
$p \to -i\hbar \frac{\partial}{\partial x}$ is

$$\hat{H} = -\hbar^2 \frac{\partial^2}{\partial x^2} + V(x,t)$$

→ we saw the Schr. eq. for a free particle:

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

- general expression; $\hat{\mathcal{H}} \psi(x,t) = i\hbar \frac{\partial}{\partial t} \psi(x,t)$

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

this is called TIME DEP. SCHRÖDINGER EQ

Class of problems

→ STATIONARY STATES:

If the potential does not dep. on t; then the Schr. eq can be solved by:

- $\Psi(x,t) = \psi(x) \cdot \phi(t)$ separation of variables $\begin{cases} (1) \text{ temporal} \\ (2) \text{ spatial} \end{cases}$

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

we can div / $\psi(x)\phi(t)$

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

each of these terms needs to be = constant

2 independent equations:

TEMPORAL PART: $i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = C$ we denote it by E

- first order diff. equation: $\phi(t) = e^{-iE/\hbar\, t}$

$$\left(\frac{E}{\hbar}\right) = [t]^{-1} = \omega \quad \rightarrow \quad C = \hbar\omega = E$$

~ freq

for the sp. part we solve: this is called TIME INDEP. SCHRÖD. eq

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

$$\downarrow$$

$$\hat{H}\psi(x) = E\psi(x)$$

→ we want to find eigenvalues and eigenstates for our operator: $\hat{H}$

Stationary state: $\Psi(x,t) = \psi(x)\, e^{\frac{-iEt}{\hbar}}$ the w.f. dep. on t

the prob. density, which is physical property: $|\Psi(x,t)|^2 = \psi^*(x)\psi(x)$ → does not dep. on t

for stationary states, the whereabouts of the particle do not change with time

Why stationary states are cool:

Classically an electron (charged particle) orbiting in an atom should constantly lose en. in the form of e.m. radiation.

In Q.M. the electron is a stationary cloud. Its prob. density is = const., its charge density is = const. its energy is a well defined const. Q.M. explains atom stability

accel. charge radiates en. Larmor formula