TDSE (1D)

$$i\hbar \frac{\partial \psi}{\partial t}(x,t) = \underbrace{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \overbrace{V(x,t)}^{\text{Real}} \right]}_{\hat{H}} \psi(x,t)$$

Assume continuity of space and time

Probability density $|\psi(x,t)|^2 = \psi^*\psi$

$$\left(\begin{array}{l}\text{Probability to find}\\ \text{the particle at}\\ \text{position } x\in[a,b]\end{array}\right) = \int_a^b dx\, |\psi(x,t)|^2$$

$\Rightarrow \psi$ has unit of $[\text{Volume}]^{-1/2}$

Normalization $\displaystyle\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2 = 1$ at any moment in time

Key theme: Linearity

Separable solutions $\Psi_n(x,t) = \psi_n(x)\,\varphi_n(t)$

Can't bring in front of $\hat{H}$

$$i\hbar\, \psi_n(x) \frac{\partial \varphi_n(t)}{\partial t} = \varphi_n(t)\, \hat{H}\, \psi_n(x)$$

$$\underbrace{\frac{1}{\varphi_n}\frac{\partial \varphi_n(t)}{\partial t}}_{\text{Function of } t} = \underbrace{-\frac{i}{\hbar}\frac{1}{\psi_n}\hat{H}\psi_n(x)}_{\text{Function of } x} \Rightarrow \text{Both sides} = \text{constant}$$

$$\frac{1}{\varphi_n}\frac{\partial \varphi_n(t)}{\partial t} = -\frac{i}{\hbar}E \Rightarrow \varphi_n(t) = e^{-iE_n t/\hbar}$$

Stationary state $\Psi_n(x,t) = \varphi_n(x)\, e^{-iE_nt/\hbar}$

C-T notation

Why stationary? $|\Psi_n(x,t)|^2 = |\varphi_n(x)|^2$ doesn't depend on time.

Linearity $\Rightarrow$ General solution can be built as linear combinations of stationary states

TISE

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\varphi_n(x) = E_n\varphi_n(x)}$$

Eigenvalue equation

De Broglie wave

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

$$E = h\nu = \hbar\omega, \qquad \omega = 2\pi\nu$$

$$\hbar = h/2\pi$$
$$= 1.05\times 10^{-34}\ \mathrm{J\cdot s}$$

$[\hbar] = [\text{Energy}][\text{Time}]$ Unit of action

$= [\text{Force}]\underbrace{[\text{Length}]}_{=[L]}\underbrace{[\text{Time}]}_{=[T]}$

$= [\text{Mass}]\dfrac{[L]}{[T]^2}[L][T]$

$= [L][\text{Momentum}]$

Photon

$$E = pc \Longleftrightarrow \omega = \frac{E}{\hbar} = \frac{pc}{\hbar} = ck$$

$$\frac{\omega}{k} = c$$

Non-relativistic

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

$$\frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{p}{2m} = \frac{v}{2}$$ (Half the classical velocity)

Phase velocity

Not group velocity! $\rightarrow$ Look at free particles

Free particle $V=0$ $\qquad -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_n = E_n\varphi_n$

$$\frac{1}{\varphi_n}\frac{d^2\varphi_n}{dx^2} = -\frac{2mE_n}{\hbar^2} = -k_n^2 \Rightarrow \begin{pmatrix}\text{L.I.}\\ \text{solutions}\end{pmatrix} = e^{\pm ik_n x} = e^{\pm ip_n x/\hbar}$$

e^{-ikx} $\qquad\qquad$ e^{ikx}

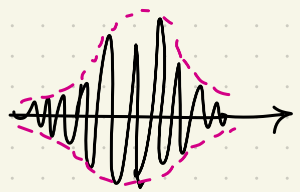
 

Left-moving $\qquad\qquad$ Right-moving

Both not normalizable $\rightarrow$ Take superpositions that are normalizable

Wave packet

$$\Psi(x,t) = \int \frac{dk}{(2\pi)^{1/2}}\,\tilde{\varphi}(k)\, e^{\overbrace{ikx - iEt/\hbar}^{i(kx-\omega t)/\hbar}}$$



$p=\hbar k$

$$= \int \frac{dp}{(2\pi\hbar^2)^{1/2}}\,\tilde{\varphi}(p)\, e^{i(px-Et)/\hbar}$$

$$\omega(k) = \underbrace{\omega(k_0)}_{/k} + (k-k_0)\underbrace{\frac{d\omega}{dk}}_{/k} + \underbrace{\frac{(k-k_0)^2}{2!}\frac{d^2\omega}{dk^2} + \dots}$$

Phase velocity

Group velocity

Why?

Dispersion

(Waves with different k move at different speeds)

$$s = k - k_0$$

$$\Psi(x,t) \approx \int \frac{ds}{\sqrt{2\pi}}\, \tilde{\varphi}(k_0+s)\, e^{i\left[(k_0+s)x - (\omega_0 + s\omega_0')\right]t}$$

$$(k_0+s)(x-\omega_0' t) = (k_0+s)x - k_0\omega_0' t - s\omega_0' t$$

$$= e^{ik_0\omega_0' t}\, e^{-i\omega_0 t} \int \frac{ds}{\sqrt{2\pi}}\, \tilde{\varphi}(k_0+s)\, e^{i(k_0+s)(x-\omega_0' t)}$$

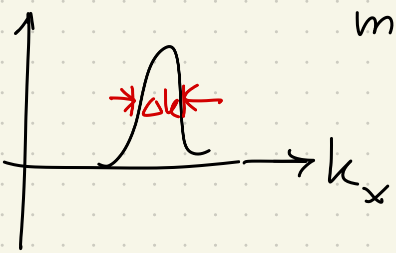
$$= e^{-i(\omega_0 - k_0\omega_0')t}\, \Psi(\underbrace{x-\omega_0' t}, 0)$$

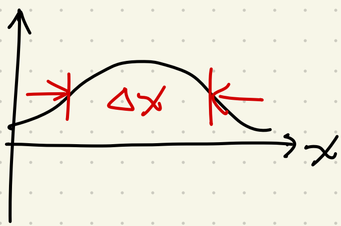
Ballistic motion with velocity

(Group velocity) $\quad \omega_0' = \left.\frac{d\omega}{dk}\right|_{k=k_0}$

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

$$\omega' = \frac{\hbar k}{m} = \frac{p}{m} = V_{classical}$$





Small $\Delta k \longleftrightarrow$ Big Δx $\qquad \Delta x\, \Delta k \gtrsim 1$

Uncertainty relation $\qquad \Delta x\, \Delta p \gtrsim \hbar$

Momentum-space wave function

$$\tilde{\Phi}(p,t) = \int \frac{dx}{\sqrt{2\pi\hbar}} \Psi(x,t)\, e^{-ipx/\hbar} \quad (\text{FT})$$

Inverse FT

$$\Psi(x,t) = \int \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \int \frac{dx'}{\sqrt{2\pi\hbar}} \Psi(x',t)\, e^{-ipx'/\hbar}$$

$$= \int dx' \, \Psi(x',t) \underbrace{\int \frac{dp}{2\pi\hbar} e^{ip(x-x')/\hbar}}_{\delta(x-x')}$$

$$= \Psi(x,t)$$

$$|\tilde{\Phi}(p,t)|^2 dp = \left(\begin{array}{c} \text{Probability to find the particle} \\ \text{having momentum within } dp \end{array} \right)$$

$$\int dp\, |\tilde{\Phi}(p,t)|^2 = 1$$

kth moment $\quad \langle \overset{\text{(classical)}}{A^k} \rangle = \int dx\, p(a)\, a^k$

Expectation value $\quad k=1$

Variance $\quad \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 - 2A\langle A \rangle + \langle A \rangle^2 \rangle$

$$= \langle A^2 \rangle - 2\langle A \rangle \langle A \rangle + \langle A \rangle^2$$

The part of the 2nd moment that is independent of the mean $\longrightarrow$ $= \langle A^2 \rangle - \langle A \rangle^2$

$$\langle p \rangle = \int dp\, p\, |\tilde{\Phi}(p,t)|^2$$

$$= \int dp\, p \int \frac{dx}{\sqrt{2\pi\hbar}} \Psi^*(x,t)\, e^{ipx/\hbar} \int \frac{dx'}{\sqrt{2\pi\hbar}} \Psi(x',t) e^{-ipx'/\hbar}$$

$$= \int dx\, \Psi^*(x,t) \int dx'\, \Psi(x',t) \int \frac{dp}{2\pi\hbar} \underbrace{p\, e^{-ip(x'-x)/\hbar}}_{-\frac{\hbar}{i}\frac{\partial}{\partial x} \underbrace{e^{-ip(x'-x)/\hbar}}_{\delta(x-x')}}$$

Integrate by parts

$$= \int dx\, \Psi^*(x,t) \int dx\, \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi(x,t)$$

$$\int dx'\, \Psi \frac{\partial}{\partial x} \delta(x-x') = \cancel{\Psi\, \delta(x-x') \Big|_{-\infty}^{\infty}}^{\,0} - \int dx\, \frac{\partial \Psi}{\partial x} \delta(x-x')$$

Regularity conditions

$$\boxed{\begin{array}{l} \varphi_n \text{ continuous and bound} \\ \varphi_n' \text{ bound} \end{array}}$$

Normalization

$\int dx\, |\varphi_n(x)|^2 = 1$ but non-normalizable states such as e^{ikx} can be useful

Remarks

1. Thermal de Broglie wavelength $\frac{h}{\sqrt{2\pi m k_B T}}$ (A_I in C-T)

2. Current associated to the probability density $|\psi(x,t)|^2$