

# Free Particle

$$H = \frac{p^2}{2m}$$

$$E_n = \frac{(\hbar k)^2}{2m} =$$

$$k = \frac{n\pi}{L} \quad \text{with } n \in \mathbb{Z}$$

$$= \frac{1}{2m} \left( \frac{n\pi\hbar}{L} \right)^2$$

$$E_{n+1} - E_n = \frac{1}{2m} \left[ \frac{(n+1)\pi\hbar}{L} \right]^2 - \frac{1}{2m} \left[ \frac{n\pi\hbar}{L} \right]^2$$

$$\Delta E = \frac{1}{L^2} \left\{ \frac{1}{2m} [(n+1)\pi\hbar]^2 - \frac{1}{2m} (n\pi\hbar)^2 \right\}$$

What happens the length  $L \rightarrow \infty$

$$\Delta E \propto \frac{1}{L^2}$$

$$\Rightarrow L \rightarrow \infty \Rightarrow \Delta E \rightarrow 0$$

Classical limit

There's no quantization

Schrödinger Eq.

$$i\hbar \partial_t \Psi = H\Psi$$

$$= -\frac{\hbar^2}{2m} \partial_x^2 \Psi(x,t)$$

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

$$p \rightarrow -i\hbar \partial_x$$

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

Separate the variables

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

$$\frac{1}{f} \frac{\partial f(t)}{\partial t} = -\frac{iE}{\hbar}$$

$$\int \frac{\partial f}{f} = -\frac{iE}{\hbar} \int dt$$

$$\Rightarrow f(t) = f_0 e^{-iEt/\hbar}$$

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

$$\frac{\partial^2}{\partial x^2} \psi(x) = -\frac{2mE}{\hbar^2} \psi(x)$$

$$= -k^2 \psi(x) \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\psi(x) = C \sin(kx) + D \cos(kx)$$

$\psi(x)$  can also be written as

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$

Find the relation between coefficients A, B and C, D.

$$\Psi(x,t) = (A e^{ikx} + B e^{-ikx}) e^{-iEt/\hbar}$$

$E$  is absorbed on A and B

$$= A e^{i(kx - Et/\hbar)} + B e^{-i(kx + Et/\hbar)}$$

very familiar from Optics

Two plane waves

towards the right

propagating

towards the left

Assumed  $k > 0$  ( $k^2 = \frac{2mE}{\hbar^2}$ )

let  $k$  take negative values:

Physical interpretation  $\rightarrow$  direction of the propagation is reversed.

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

$$\omega = E/\hbar$$

Check that  $\omega$  has dimensions of a frequency!

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = |A|^2 \int_{-\infty}^{\infty} |e^{i(kx - \omega t)}|^2 dx = |A|^2 \int_{-\infty}^{\infty} dx$$

$$= 2|A|^2 \infty = \infty$$

The free-particle is unphysical!

What happens if we take a sum over many frequencies (or  $k$  values)?

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \Rightarrow \psi(x) = \sum_n a_n \psi_n(x)$$

also a solution to the Schrödinger Eq.

$$E_n = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2$$

$$\sum_n \Leftrightarrow \sum_k$$

over the allowed values of  $k$ .

For the free particle  $E = \frac{\hbar^2 k^2}{2m}$  is not restrained

$\sum_k$   
discrete  
set  
of values

$\rightarrow \int dk$   
continuous  
set of values

$$\psi(x,t) = \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \omega t)} dk$$

what happens with this state?

$\phi(k)$ : the weight of each  $k$ -value into the  $\psi(x,t)$

$$\int_{-\infty}^{\infty} dx |\psi(x,t)|^2 = \int_{-\infty}^{\infty} dx \psi^*(x,t) \psi(x,t)$$

$$\psi^*(x,t) = \int_{-\infty}^{\infty} \phi^*(q) e^{-i(qx - \omega t)} dq$$

$$\psi(x,t) = \int_{-\infty}^{\infty} dk \phi(k) e^{i(kx - \omega t)}$$

$$\psi^* \psi = \int_{-\infty}^{\infty} \phi^*(q) e^{-i(qx - \omega t)} dq \int_{-\infty}^{\infty} dk \phi(k) e^{i(kx - \omega t)}$$

indep. of  $k$                       indep. of  $q$

$$= \int_{-\infty}^{\infty} dk \phi(k) \int_{-\infty}^{\infty} dq \phi^*(q) e^{i(kx - \omega t - qx + \omega t)}$$

$$= \int_{-\infty}^{\infty} dk \phi(k) \int_{-\infty}^{\infty} dq \phi^*(q) e^{i(k-q)x}$$

$$\int_{-\infty}^{\infty} dx |\psi(x,t)|^2 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dk \phi(k) \int_{-\infty}^{\infty} dq \phi^*(q) e^{i(k-q)x}$$

ind. of  $x$

$$= \int_{-\infty}^{\infty} dk \phi(k) \int_{-\infty}^{\infty} dq \phi^*(q) \int_{-\infty}^{\infty} dx e^{i(k-q)x}$$

$\delta(k-q)$ : Dirac delta function

$$\int_a^b f(x) \delta(x-x_0) dx = \begin{cases} f(x_0) \\ 0 \end{cases} \quad \text{if } \underline{a} < x_0 < \underline{b}$$

otherwise

$$\int_{-\infty}^{\infty} dx |\psi(x,t)|^2 = \int_{-\infty}^{\infty} dk \phi(k) \int_{-\infty}^{\infty} dq \phi^*(q) \delta(k-q)$$

$q=k$

$$= \int_{-\infty}^{\infty} dk \phi(k) \phi^*(k)$$

$$\int_{-\infty}^{\infty} dx |\psi(x,t)|^2 = \int_{-\infty}^{\infty} dk |\phi(k)|^2 = 1$$

$$\rightarrow \psi(x,t) = \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \omega t)} dk \quad \text{Is physical}$$

All the results that we know from optics apply here!

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

$$E = \hbar \omega$$

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

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

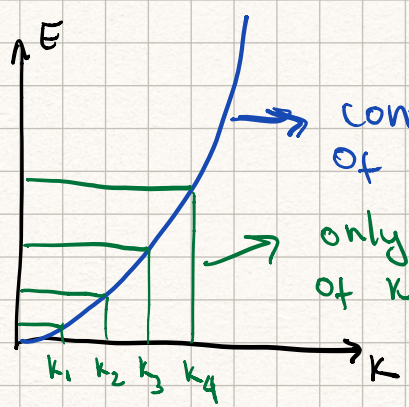
Dispersion relation

$v_\phi$ : phase velocity

$$v_\phi = \frac{\omega}{k} = \frac{\hbar k}{2m}$$

$v_g$ : group velocity

$$v_g = \frac{\partial \omega}{\partial k} = \frac{\hbar k}{m}$$



continuum of values of free particle

only some values of k are allowed of particle in a box

$\phi(k)$ :