# Free particle

$V(x) = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

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

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

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

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

$$= A e^{ikx} e^{-i\hbar k^2 t/2m} + B e^{-ikx} e^{-i\hbar k^2 t/2m}$$

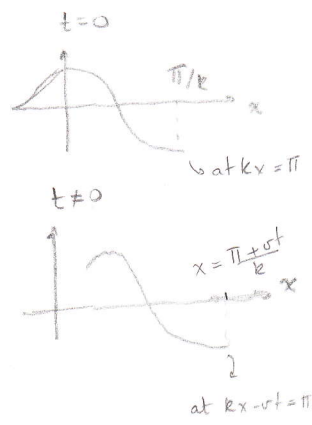
$$= A e^{ik\left(x - \underbrace{\frac{\hbar k}{2m}}_{v_{ph}} t\right)} + B e^{-ik\left(x + \underbrace{\frac{\hbar k}{2m}}_{v_{ph}} t\right)}$$

$\boxed{x \pm v_{ph} t}$ → shape does not change

$A e^{ik(x - v_{ph} t)}$ → wave moving to the right with $v_{ph}$

$B e^{-ik(x + v_{ph} t)}$ → wave moving to the left with $v_{ph}$

Example $\begin{cases} \text{moving to the right} \\ \cos(kx - vt) \end{cases}$




$$= A e^{ik\left(x - \frac{\hbar k}{2m} t\right)}$$

(plane wave)

$\begin{cases} k \oplus \rightarrow \text{left} \\ k \ominus \rightarrow \text{right} \end{cases}$

$$v_{ph} = v_{quantum} = \frac{\hbar k}{2m}$$
(speed of wave)

BUT

$$v_{clas} = \frac{\hbar k}{m}$$

$$\left.\begin{aligned} E &= \frac{1}{2} m v^2 \\ E &= \frac{\hbar^2 k^2}{2m} \end{aligned}\right\} \quad v = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2\hbar^2 k^2}{2m^2}}$$

→) Free particle cannot exist in a stationary state

→) Each stationary state is NOT physically realizable

↓

is NOT normalizable

$$\int_{-\infty}^{\infty} \psi_k^* \psi_k \, dx = |A|^2 \int_{-\infty}^{\infty} dx = |A|^2 \infty \quad (!)$$

→) but stationary states form a complete set

general solution of time dep. Schröd. eq. – linear combination of $\psi_k(x,t)$

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i k \left(x - \frac{\hbar k}{2m} t\right)} dk}$$

→ WAVE PACKET

$\int$ because $k, p \to$ continuous

$$\left(p = \frac{h}{\lambda}, \; k = \frac{2\pi}{\lambda} \Rightarrow p = \hbar k\right)$$

$$\frac{\phi(k)}{\sqrt{2\pi}} \leftrightarrow c_n$$

$v_{ph} \to$ phase velocity / velocity of each wave

$v_{clas} = v_g \to$ group velocity / velocity of the group of waves / same velocity of the particle

$$v_{ph} = \frac{\omega}{k} \qquad v_g = \frac{d\omega}{dk}$$

Modern Physics example

$$\sin(kx - \omega t) + \sin\left((k + dk)x - (\omega + d\omega)t\right)$$

$$\propto \underbrace{\sin(kx - \omega t)}_{} \; \underbrace{\cos\left(\frac{dk}{2} x - \frac{d\omega}{2} t\right)}_{\text{envelope}}$$

↳ group velocity

infinite square well

$$\Psi(x,0) = \sum c_n \psi_n(x) \Rightarrow \int \psi_m^* \Psi(x,0)\,dx = \sum c_n \underbrace{\int \psi_m^* \psi_n\,dx}_{\delta_{nm}}$$

Kronecker delta

discrete

a) To find $\phi(k)$ we need $\Psi(x,0)$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ikx}\, dk$$

$$\frac{1}{\sqrt{2\pi}} \int e^{-ik'x}\, \Psi(x,0)\, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, \phi(k) \int_{-\infty}^{\infty} dx\, e^{ix(k-k')}$$

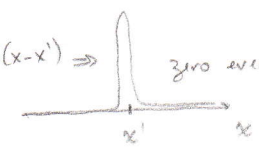
$\delta(k-k')$ ← delta function

continuous analogue of Kronecker delta

delta function

$$\boxed{\begin{aligned} \delta(x-x') &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iu(x-x')}\, du \\ f(x') &= \int_{-\infty}^{\infty} \delta(x-x')\, f(x)\, dx \end{aligned}}$$

$\delta(x-x') \Rightarrow$




zero everywhere, except at $x = x'$

$$\int_{-\infty}^{\infty} \delta(x)\, dx = 1$$

$$\int_{x'-\epsilon}^{x'+\epsilon} \delta(x-x')\, f(x)\, dx = f(x')$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik'x}\, \Psi(x,0)\, dx = \int_{-\infty}^{\infty} dk\, \phi(k)\, \delta(k-k') = \phi(k')$$

$$\boxed{\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx}\, \Psi(x,0)\, dx}$$

Fourier transform

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk$$ → $f(x)$ is the inverse Fourier transform of $F(k)$

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$ → $F(k)$ is the Fourier transform of $f(x)$

Example 2.6 Free particle is initially localized

$$\Psi(x,0) = \begin{cases} A & -a < x < a \\ 0 & \text{otherwise} \end{cases}$$

Find $\Psi(x,t)$ $\begin{cases} \text{1st) normalization (find A)} \\ \text{2nd) given } \Psi(x,0)\text{, find } \phi(k) \\ \text{3rd) write } \Psi(x,t) \end{cases}$

$$|A|^2 \int_{-a}^{a} dx = 1 \Rightarrow |A|^2\, 2a = 1 \Rightarrow A = \frac{1}{\sqrt{2a}}$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0)\, e^{-ikx}\, dx = \frac{1}{2\sqrt{a\pi}} \int_{-a}^{a} e^{-ikx}\, dx$$

$$= \frac{1}{2\sqrt{a\pi}} \frac{e^{-ika} - e^{+ika}}{(-ik)} = \frac{1}{\sqrt{a\pi}} \frac{1}{k} \frac{(e^{ika} - e^{-ika})}{2i} = \frac{1}{\sqrt{\pi a}} \frac{\sin ka}{k}$$

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2a}\,\pi} \int_{-\infty}^{\infty} \frac{\sin ka}{k}\, e^{ik\left(x - \frac{\hbar k}{2m} t\right)}\, dk}$$

can only solve numerically

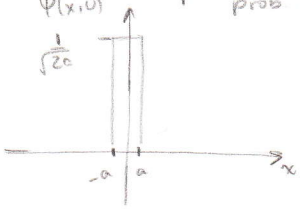
limiting cases

a) a is very small

$$\Psi(x,0) = \frac{1}{\sqrt{2a}}$$

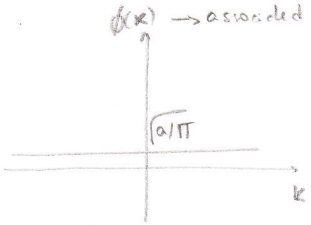
$$\frac{\sin ka}{k} \sim \frac{ka}{k} = a \Rightarrow \phi(k) \frac{a}{\sqrt{\pi a}} \Rightarrow \boxed{\phi(k) = \sqrt{\frac{a}{\pi}}}$$

$\Psi(x,0) \rightarrow$ associated with prob for position




(peaked)

$\phi(k) \rightarrow$ associated with prob for momentum



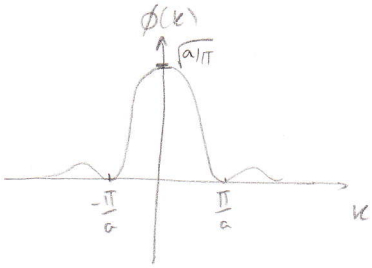

(flat)

spread in position is small $\Rightarrow$ spread in momentum is large

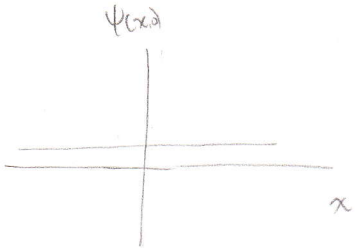
a) a is very large

$\frac{\sin Ka}{Ka}$ $\begin{cases} \text{at } Ka = 0 \rightarrow \text{maximum} \\ \text{at } Ka = \pm\pi \rightarrow \text{zero} \end{cases}$

$$\phi(k) = \frac{\sin Ka}{Ka}\sqrt{\frac{a}{\pi}}$$




$\begin{cases} \rightarrow) \; Ka \sim 0 \\ \Downarrow \\ \boxed{\phi(k) = \sqrt{a/\pi}} \\ \\ \rightarrow) \; Ka = \pm\pi \\ \boxed{\phi(k) = 0} \end{cases}$




$$\psi(x,0) = \frac{1}{\sqrt{2a}}$$

$\begin{cases} \text{momentum is localized} \\ \text{position is spread} \end{cases}$

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$v_{ph}$ may be $\neq$ from $\frac{p}{m}$

$v_{ph}$ → phase velocity → velocity of $\psi_k$

$\frac{p}{m}$ → group velocity → velocity of the wave packet

$\left.\begin{matrix}\text{group} \\ \text{velocity}\end{matrix}\right\}$ = to the speed of the particle it represents

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ik\left(x - \frac{\hbar k}{2m} t\right)}\, dk$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx - \omega t)}\, dk \longrightarrow \boxed{v_{phase} = \frac{\omega}{k}}$$

$$\boxed{\omega = \frac{\hbar k^2}{2m}} \longleftarrow \text{dispersion relation}$$

Assume

$\phi(k)$ peaked around $k_0$

$$\omega(k) \simeq \omega_0 + \omega_0'(k - k_0)$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx - \omega_0 t - \omega_0'(k-k_0)t)}\, dk$$

$k - k_0 = s$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k_0 + s)\, e^{i(k_0 x + sx - \omega_0 t - \omega_0' s t)}\, ds$$

$$= \frac{1}{\sqrt{2\pi}}\, e^{i(-\omega_0 t + k_0 \omega_0' t)} \int \phi(k_0 + s)\, e^{i(k_0 + s)(x - \omega_0' t)}\, ds$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int \phi(k_0 + s)\, e^{i(k_0 + s)x}\, ds$$

$$\Psi(x,t) = \underbrace{e^{-i(\omega_0 t - k_0 \omega_0' t)}}_{\text{phase factor}}\, \Psi(x - \omega_0' t, 0) \longrightarrow \boxed{v_{group} = \frac{d\omega}{dk}}$$

$$\boxed{v_{phase} = \frac{\omega}{k}}$$

$\omega = \frac{\hbar k^2}{2m} \Rightarrow v_{particle} = v_{group} = \frac{\hbar k}{m} = 2\, v_{phase}$

Prob. 2.22 Free particle with initial wave function

$$\Psi(x,0) = A e^{-ax^2}$$

a) $$\int_{-\infty}^{\infty} |\Psi(x,0)|^2 \, dx = 1 \Rightarrow |A|^2 \int_{-\infty}^{\infty} e^{-2ax^2} \, dx = |A|^2 \sqrt{\frac{\pi}{2a}} \Rightarrow A = \left(\frac{2a}{\pi}\right)^{1/4}$$

b) Find $\Psi(x,t)$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \, e^{i\left(kx - \frac{k^2\hbar}{2m} t\right)} \, dk$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} \, e^{-ikx} \, dx$$

<u>complete the square</u>

trying to put in the form $(x^2 + 2Bx + B^2) = (x+B)^2$

$$-ax^2 - ikx = -a\left(x^2 + \frac{2ikx}{2a}\right) = -a\left(x^2 + \frac{2ikx}{2a} - \frac{k^2}{4a^2}\right) - \frac{k^2}{4a}$$

$$= -a\left(x + \frac{ik}{2a}\right)^2 - \frac{k^2}{4a}$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-a(x+ik/2a)^2} \, e^{-k^2/4a} \, dx$$

$$s = x + ik/2a$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-as^2} \, e^{-k^2/4a} \, ds = \frac{1}{\sqrt{2\cancel{\pi}}} \left(\frac{2a}{\pi}\right)^{1/4} \sqrt{\frac{\cancel{\pi}}{a}} \, e^{-k^2/4a}$$

$$= \frac{1}{(2a\pi)^{1/4}} e^{-k^2/4a}$$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \frac{1}{(2a\pi)^{1/4}} \int_{-\infty}^{\infty} e^{-k^2/4a} \, e^{i\left(kx - \frac{k^2\hbar}{2m}t\right)} \, dk$$

$$-\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)\underbrace{\left[k^2 - \frac{2}{2}\frac{ikx}{\left(\frac{1}{4a}+\frac{i\hbar t}{2m}\right)} - \frac{x^2}{4\left(\frac{1}{4a}+\frac{i\hbar t}{2m}\right)^2}\right]}_{\underbrace{\left(k - \frac{ix}{2\left(\frac{1}{4a}+\frac{i\hbar t}{2m}\right)}\right)^2}_{s}} - \frac{x^2}{4\left(\frac{1}{4a}+\frac{i\hbar t}{2m}\right)}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(2a\pi)^{1/4}} \int_{-\infty}^{\infty} e^{-\left(\frac{1}{4a}+\frac{i\hbar t}{2m}\right)s^2} \, e^{-\frac{x^2}{\left(\frac{1}{a}+\frac{i2\hbar t}{m}\right)}} \, ds$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(2a\pi)^{1/4}} \underbrace{\frac{\sqrt{\pi}}{\sqrt{\frac{1}{4a}+\frac{i\hbar t}{2m}}}}_{\underbrace{\frac{2\sqrt{a}}{\sqrt{1+\frac{2ia\hbar t}{m}}}}_{\left(\frac{\cancel{16}^{\,2}}{\cancel{4}\cdot\cancel{2}}\right)^{1/4}\left(\frac{1}{\pi}\right)^{1/4}\left(\frac{a^{\cancel{2}}}{\cancel{2}}\right)^{1/4}\frac{1}{\sqrt{1+\frac{2ia\hbar t}{m}}}}} \underbrace{e^{-x^2/\left(\frac{1}{a}+\frac{i2\hbar t}{m}\right)}}_{e^{-ax^2/\left(1+2i\frac{a\hbar t}{m}\right)}}$$

$$= \boxed{\left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{1+\frac{2ia\hbar t}{m}}} \exp\left(\frac{-ax^2}{1+\frac{2ia\hbar t}{m}}\right)}$$

c) $|\Psi(x,t)|^2$

$$= \left(\frac{2a}{\pi}\right)^{1/2} \frac{1}{\sqrt{\left(1 + \frac{4a^2\hbar^2t^2}{m^2}\right)}} \; e^{\frac{-ax^2\left(1+2ia\hbar t/m\right) - ax^2\left(1-2ia\hbar t/m\right)}{\left(1+4a^2\hbar^2t^2/m^2\right)}}$$

$$w = \sqrt{\frac{a}{1+(2\hbar a t/m)^2}} \quad \Rightarrow \quad 1 + (2\hbar a t/m)^2 = \frac{a}{w^2}$$

$$= \left(\frac{2\cancel{a}}{\pi}\right)^{1/2} \frac{w}{\sqrt{\cancel{a}}} \; e^{-2ax^2\frac{w^2}{a}} = \boxed{\sqrt{\frac{2}{\pi}}\; w\; e^{-2w^2x^2}}$$

$t$ increases $\Rightarrow$ $w$ decreases $\Rightarrow$ $|\Psi|^2$ decreases and broadens