Lecture 9

The free particle: V(x) = 0 everywhere.

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

We introduce $k \equiv \frac{\sqrt{2mE}}{\hbar}$: $\boxed{\frac{d^2\psi}{dx^2} = -k^2\psi}$

(Same as inside of infinite square well, where potential is zero.) We will write solution in exponential form instead of sin or cos.

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

There are no boundary conditions to restrict the values of the energy here, and the free particle can have any positive energy. The wave function is

$$\psi(x,t) = Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x + \frac{\hbar k}{2m}t\right)} \quad (E.1)$$

(We added $e^{-iEt/\hbar}$, $E = \frac{\hbar k}{2m}k$).

Note that in Eq. (E.1) $x \pm \frac{\hbar k}{2m}t \rightarrow x \pm vt$

where v is a constant . Therefore, $\psi(x,t)$ represents a wave of fixed profile that travels with speed v in the direction of ±x. Every point on the wave form is moving with the same speed, so the shape does not change as it propagates.

The only difference is in the sign of k.

$$\psi(x,t) = \underbrace{Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)}}_{\text{wave moving to the right}} + \underbrace{Be^{-ik\left(x + \frac{\hbar k}{2m}t\right)}}_{\text{wave moving to the left}}$$

Therefore, we can put these two expressions together and allow k to be both positive and negative.

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

$$k = \pm \frac{\sqrt{2mE}}{\hbar}, \text{ with } \begin{cases} k > 0 & \text{traveling to the right} \\ k < 0 & \text{traveling to the left} \end{cases}$$

These are "stationary states" of the free particle, that are propagating waves with wavelength

$$\lambda = \frac{2\pi}{|k|}.$$

According to de Broglie formula, the corresponding momentum is

$$p = \frac{2\pi\hbar}{\lambda} \Rightarrow p = \hbar k.$$

The corresponding speed of such waves is

$$v_{quantum} = \frac{\hbar |k|}{2m} = \sqrt{\frac{E}{2m}}$$

just from looking at the coefficient $x \pm vt$ in Eq. (E.1) on the previous page.

Note that the classical speed of the free particle with energy E is obtained from

$$E = E_{kinetic} = \frac{1}{2} m v^2 \Rightarrow$$

$$v_{classical} = \sqrt{\frac{2E}{m}} = 2 v_{quantum}.$$

Therefore, it appears that the wave function travels at only half the speed of the particle that it is supposed to represent! We will return to this problem later.
The other problem is that the resulting wave function is not normalizable.

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

What does it mean? It means that the stationary states that we described do not represent physically realizable states, i.e. there can be no free particle with definite energy.
We are still interested in these states for the same reason as before: the general solution is a linear combination of stationary states. Since k is continuous, the resulting expression is an integral.

$$\underset{\substack{\uparrow \\ \text{general} \\ \text{solution}}}{\Psi(x,t)} = \underset{\substack{\uparrow \\ \text{just for convinience}}}{\frac{1}{\sqrt{2\pi}}} \int_{-\infty}^{\infty} \phi(k)\, e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}\, dk$$

$\boxed{\frac{1}{\sqrt{2\pi}}\phi(k)\,dk \text{ plays role of } c_n}$

For appropriate $\phi(k)$,this wave function can be normalized. Now it does not have a single value of E_k associated with it, but a range of values of energies and speeds.
We call it a wave packet.

If we know the initial wave function at time t=0

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

we can determine the function $\phi(k)$ (and, therefore $\Psi(x,t)$), by

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

Plancherel's theorem:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk \iff F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$

Fourier transform of $f(x)$

Inverse Fourier transform of F(k)

Note: the integrals have to exist.

Example

A free particle that is initially localized in the range $-a < x < a$ is released at time t=0:

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

where A and a are positive real constants. Find $\Psi(x,t)$.

Solution

Normalization:

$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = |A|^2 \int_{-a}^{a} dx = 2a\,|A|^2$$

$$A = \frac{1}{\sqrt{2a}}$$

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

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} \frac{1}{\sqrt{2a}} e^{-ikx} dx = \frac{1}{2\sqrt{\pi a}} \left. \frac{e^{-ikx}}{-ik} \right|_{-a}^{a}$$

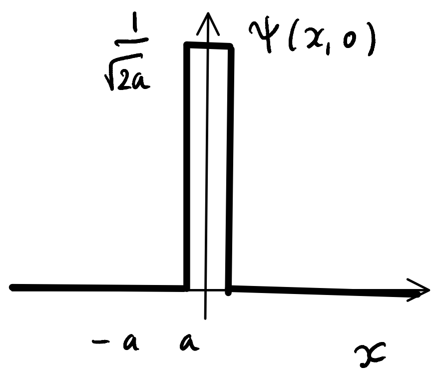
$$= \frac{1}{\sqrt{\pi a}} \frac{1}{k} \left(\frac{e^{ika} - e^{-ika}}{2i} \right) = \frac{1}{\sqrt{\pi a}} \frac{\sin(ka)}{k}$$

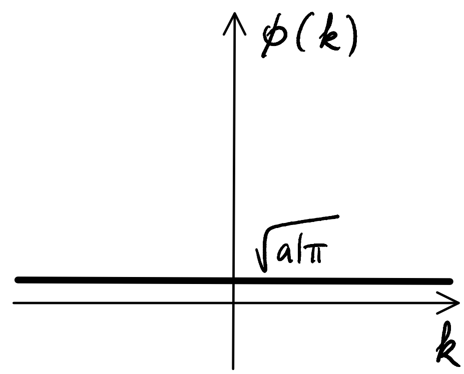
$$\Psi(x,t) = \frac{1}{\pi\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin(ka)}{k} e^{i\left(kx - \frac{\hbar k^2}{2m}\right)t} dk$$

This integral needs to be evaluated numerically.

Limiting case 1: a is very small (localized spike)

$$\sin(ka) \simeq ka \quad \text{and} \quad \phi(k) \simeq \sqrt{\frac{a}{\pi}}$$



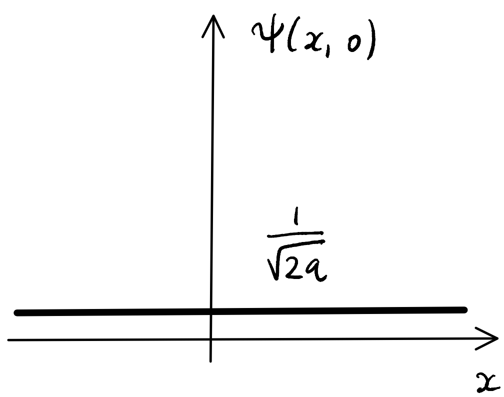


Spread in position is small, then (Example of the uncertainty principle).

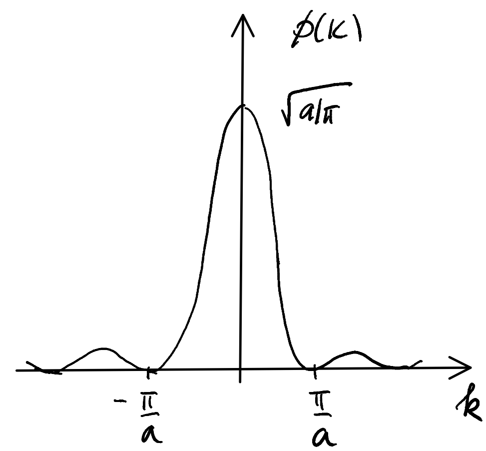
spread in momentum is large.

$(p = \hbar k)$

Limiting case 2 : large a

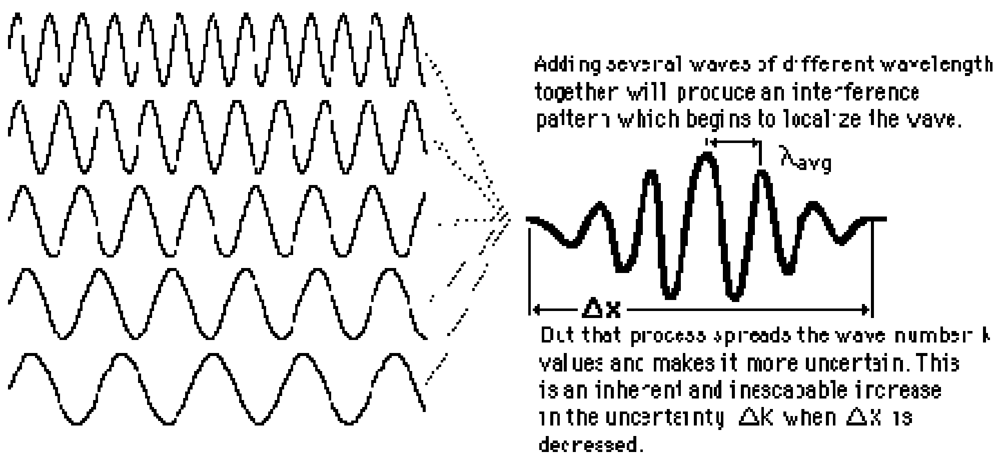


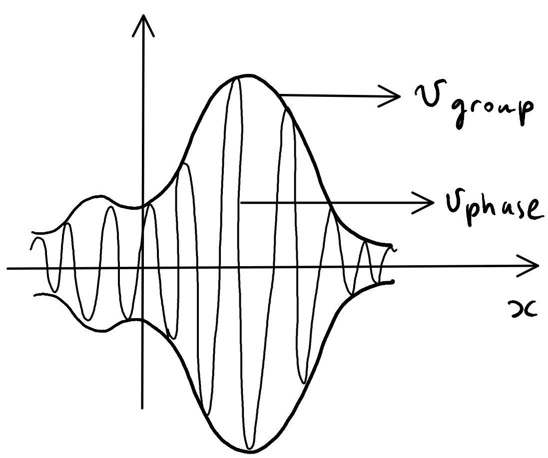
Spread in position is large



Momentum is well-defined

Now we return to the issue of velocity. First, there is really no problem because separable solutions are not physically realizable. The wave packet is a superposition of sinusoidal functions with their amplitudes modulated by ϕ. It can be visualized as "ripples" inside an "envelope". The speed of envelope (group velocity) corresponds to the particle velocity. What we found earlier was a speed of individual ripples (phase velocity).





A wave packet

Wave packet:

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

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

Group velocity

$$v_{group} = \frac{d\omega}{dk}$$

(see textbook, page 65 for derivation).

Phase velocity

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

In our case, $v_{group} = \dfrac{d\omega}{dk} = \dfrac{2\hbar k}{2m} = \dfrac{\hbar k}{m}$

$v_{phase} = \dfrac{\omega}{k} = \dfrac{\hbar k}{2m}$ and $v_{classical} = v_{group} = 2 v_{phase}$.