LECTURE 9: Wave Packets

Goal of the lecture: describe the wave function of a quantum particle using wave packets

What I expect you to learn:

- what are waves packets
- what is the group and phase velocities of wave packets
- what are Fourier Transforms
- how to express the wave function in momentum space
- how to calculate Fourier Transforms

(This roughly corresponds to section 2.4, appendix A of textbook)

A quick recap

→ We related wave-type quantities to a particle's energy and momentum:

$$p = k\hbar$$
$$E = \hbar\omega$$

→ For a free particle we have: $E = \frac{p^2}{2m} = \frac{mv^2}{2}$

which means we the following relation between ω and k:

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

→ we found an equation that obeyed this relation:

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar\frac{\partial \psi}{\partial t}}$$

A simple solution to this equation is

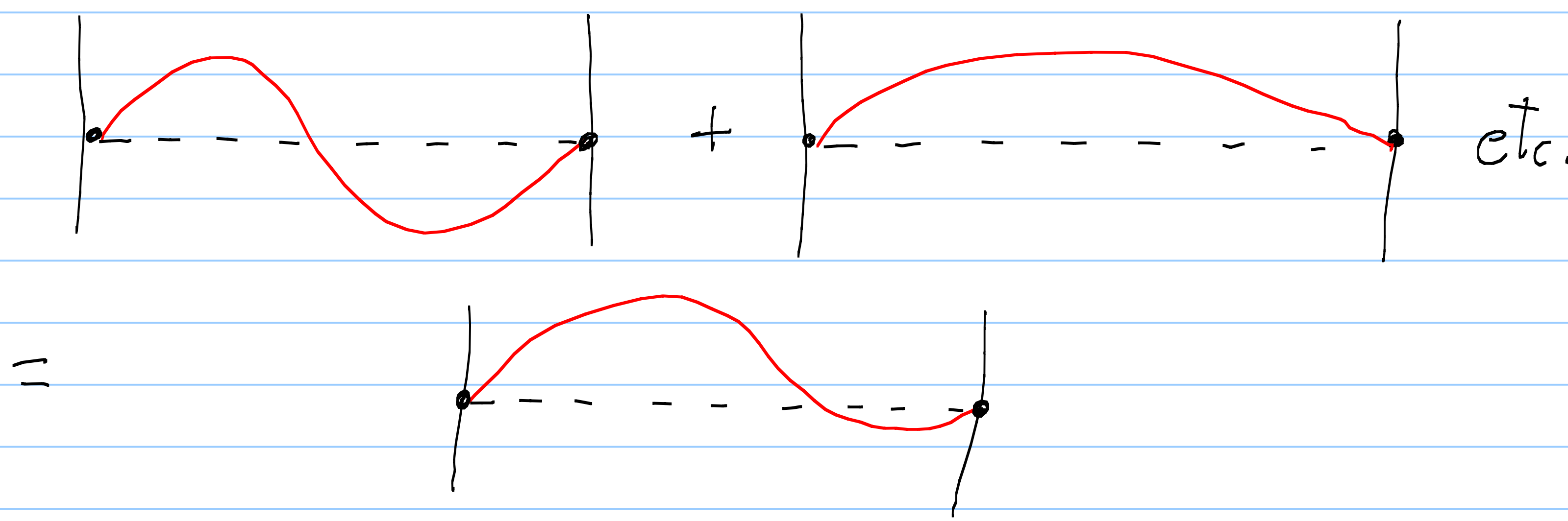
$$\psi(x,t) = A\, e^{i(kx-\omega t)}$$

A quick recap (cont.)

- we saw that in order to account for interference effects, we must be able to superimpose wave functions e.g.

$$\psi = c_1 \psi_1 + c_2 \psi_2 + \ldots \text{(superposition principle)}$$

- As a first step on our way to superimposing wave functions, we considered the superposition of sine waves in the case of a string attached at two ends:



A QUICK RECAP (CONT.)

- WE SAW THAT WE COULD EXPRESS AN ARBITRARY WAVE FORM ON THE STRING AS A SUM OF SINE AND COSINE WAVES i.E A FOURIER SERIES:

(1) $$F(x) = \frac{A_0}{2} + \sum_{n=1}^{\infty} A_n \sin nx + \sum_{n=1}^{\infty} B_n \cos nx$$

FOR EXAMPLE WE SAW:

we found the amplitudes for this example

note that (1) has discret values of K

We need To work with a continuum of K values

Wave Functions for Fixed p

For a fixed momentum, we have

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

Note that

$$\boxed{-i\hbar \frac{\partial}{\partial x}}\,\Psi = p\Psi \quad , \quad \boxed{i\hbar \frac{\partial}{\partial t}}\,\Psi = E\Psi$$

differential operators

Probability interpretation of $|\Psi|^2 \Rightarrow$

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

The plane wave cannot be normalized to unity

WAVE PACKETS IN 1 DIMENSION

WE NEED TO SUM PLANE WAVES... THE MOST GENERAL EXPRESSION IS:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \varphi(p)\, e^{i/\hbar (px - Et)}\, dp$$

↳ Amplitude for wave of momentum p (or $\hbar k$) → can be complex

Assume that $\varphi(p)$ is peaked about $p = p_0$
i.e. falls to 0 outside $[p_0 - \Delta p, p_0 + \Delta p]$

Take $\beta(p) = px - Et$

$|\psi(x,t)|$ will be largest when $\beta(p)$ is almost constant around $p = p_0$

→ remember $e^{i\theta} = \cos\theta + i\sin\theta$

$\Rightarrow$ get max of $|\psi(x,t)|$ when $\frac{d\beta}{dp} \simeq 0$

WAVE PACKETS (CONT.)

→ The max of $|\Psi(x,t)|$ will correspond to the center of the wave packet

We have $E = \frac{p^2}{2m}$, $B = px - Et$

$$\frac{dB}{dp} = x - \frac{p}{m}t = x - vt = 0$$

$$x = vt$$

$\hookrightarrow v_g$

v_g : velocity of the group of plane waves

$v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$, v_p = velocity of plane waves

$$A e^{i(kx - \omega t)} = A e^{ik(x - \frac{\omega}{k}t)} \Rightarrow v_p = \frac{\omega}{k}$$

Let's take a look here:

http://webphysics.davidson.edu/Applets/superposition/GroupVelocity.ht

WAVE PACKETS (CONT.)

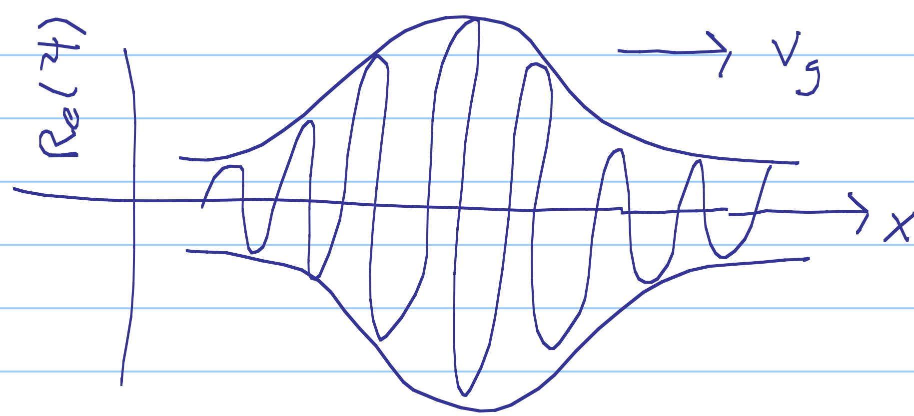
WE CAN EXPAND $E(p)$ ABOUT p_0 → TAYLOR EXPANSION

$$E(p) = p^2/2m$$

$$E(p) = E(p_0) + (p-p_0)\left.\frac{dE(p)}{dp}\right|_{p=p_0} + \frac{1}{2}(p-p_0)^2 \left.\frac{d^2E(p)}{dp^2}\right|_{p=p_0} + \ldots$$

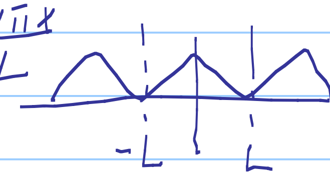
$$= \frac{p_0^2}{2m} + (p-p_0)\frac{p_0}{m} + \underbrace{\frac{(p-p_0)^2}{2m}}_{\text{neglect : } \Delta p^2 t \ll 1} + \ldots$$

$$\psi(x,t) = \underbrace{e^{\frac{i}{\hbar}(p_0 x - E(p_0)t)}}_{\text{plane wave}} \cdot \underbrace{\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{i(px - p_0)(x - v_g t)/\hbar}\,\phi(p)\,dp}_{\text{envelope function}}$$



FOURIER TRANSFORM INTERLUDE

$$F(x) = \frac{1}{2} A_0 + \sum_{n=1}^{\infty} A_n \sin\frac{n\pi x}{L} + B_n \cos\frac{n\pi x}{L}$$



we can also write:

$$F(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} C_n e^{in\pi x/L}$$

For non-periodic functions we take $L \to \infty$

as $L \to \infty$, differences between terms in the series become smaller:

$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} C_n e^{in\pi x/L} \, dn$$

let $k = n\pi/L$ and $g(k) = \frac{L C_n}{\pi}$, $dk = dn \cdot \frac{\pi}{L}$

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

Fourier Transforms (cont.)

Physically what does this all mean?

For $T = 0$, we have

* $$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \varphi(p)\, e^{ipx/\hbar}\, dx$$

→ probability amplitude for finding particle at x

→ sum of plane waves with amplitude $\varphi(p)$

* $$\varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx}\, dx$$

→ probability amplitude for finding particle with momentum p

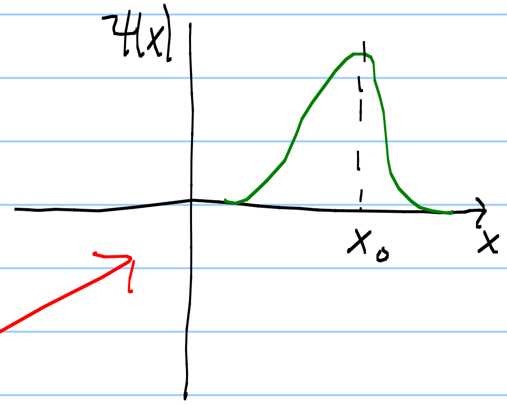
→ sum of plane waves with amplitude $\psi(x)$

→ momentum space wave function

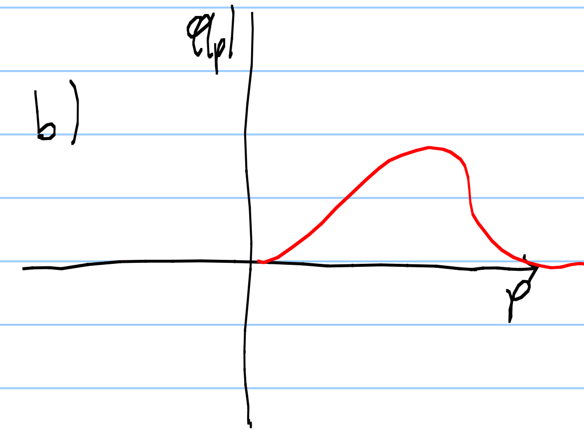
Fourier Transforms (cont.)

at $T=0$

a)



b)



For a particle whose prob. amplitude dist. looks like this, what are the amplitudes of its component plane waves?

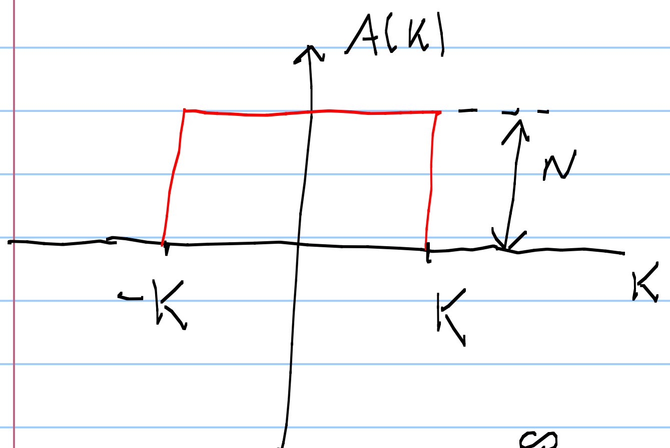
AT $T=0$, the particle is most probably at x_0 and it's velocity is given by the group velocity:

$$v_g = \left. \frac{dE}{dp} \right|_{x=x_0}$$

Fourier Transform Examples

Example 1:

We have a wave packet for which:

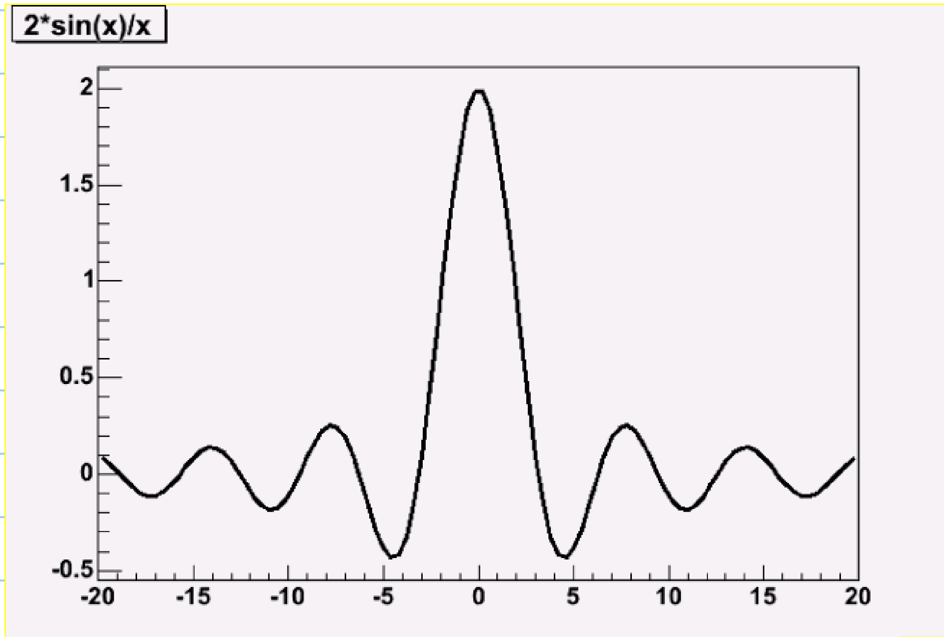


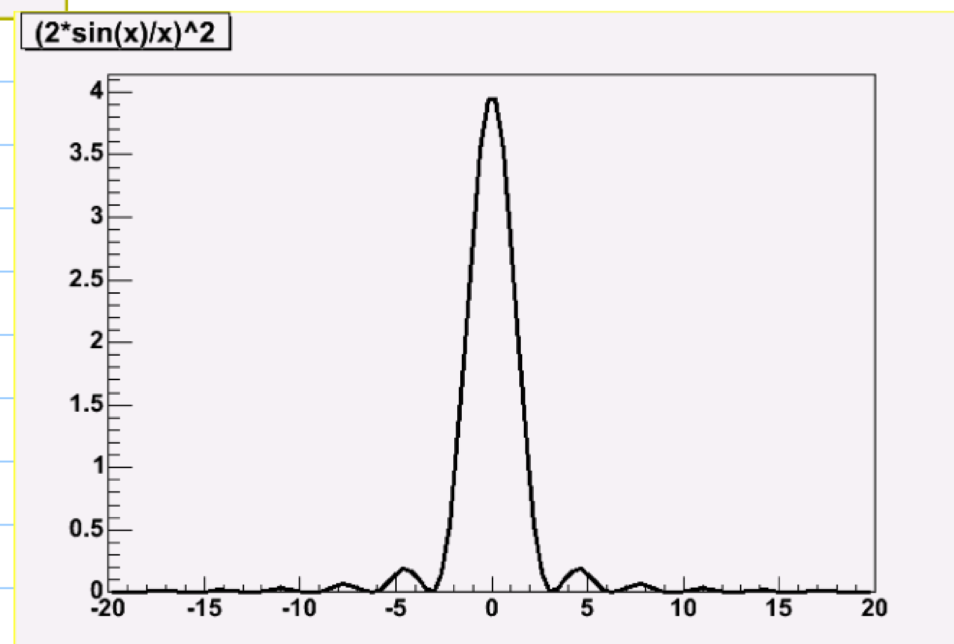
$$A(k) = N \quad \text{for } -K \le k \le K$$
$$\;\;\;\;\;\;= 0 \quad\quad k > |K|$$

$\rightarrow$ let's calculate $\psi(x,0)$

$$\psi(x,0) = \int_{-\infty}^{\infty} A(k)\, e^{ikx}\, dk = \int_{-K}^{+K} N e^{ikx}\, dk$$

$$= \frac{N}{ix}\left(\underbrace{e^{iKx}}_{\text{big } K} - \underbrace{e^{-iKx}}_{\text{big } K}\right) = 2N\,\frac{\sin Kx}{x}\;:$$

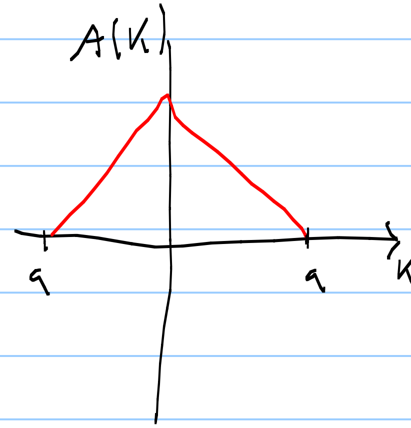

2*sin(x)/x
2
1.5
1
0.5
0
-0.5
-20
-15
-10
-5
0
5
10
15
20


(2*sin(x)/x)^2
4
3.5
3
2.5
2
1.5
1
0.5
0
-20
-15
-10
-5
0
5
10
15
20

Fourier Transform Examples

Example 2:

We have a wave packet for which:



$$A(K) = \begin{cases} A \cdot (a - |K|), & |K| \leq a \\ 0, & |K| > a \end{cases}$$

real

positive

→ Find A such that $A(K)$ is normalised:

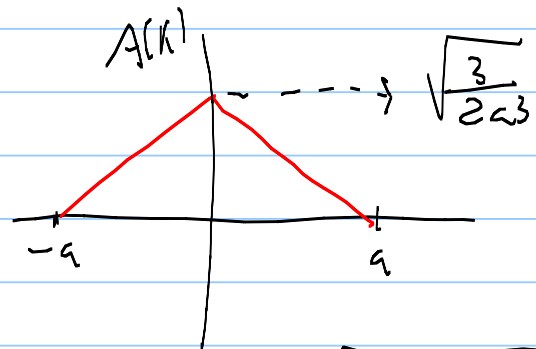
$$1 = \int_{-\infty}^{\infty} |A(K)|^2 \, dK = A^2 \int_{-a}^{0} (a+K)^2 \, dK + A^2 \int_{0}^{a} (a-K)^2 \, dK$$

$$= 2A^2 \int_0^a (a-K)^2 \, dK = 2A^2 \int_0^a (a^2 - 2aK + K^2) \, dK$$

$$= 2A^2 \cdot \left(a^2 K - a K^2 + \frac{K^3}{3} \right) \Big|_0^a = 2A^2 \cdot \left(a^3 - a^3 + \frac{a^3}{3} \right) = \frac{2}{3} a^3 \cdot A^2$$

Example 2 continued:

$$1 = \frac{2a^3}{3} A^2 \Rightarrow A = \sqrt{\frac{3}{2a^3}}, \quad A(K) = \sqrt{\frac{3}{2a^3}}\,(a - |K|)$$



The Transform is then:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(K)\, e^{iKx}\, dK$$

$$\Rightarrow \frac{1}{\sqrt{2\pi}} \cdot \sqrt{\frac{3}{2a^3}} \left[\int_{-a}^{0} (a+K)\, e^{iKx}\, dK + \int_{0}^{a} (a-K)\, e^{iKx}\, dK \right]$$

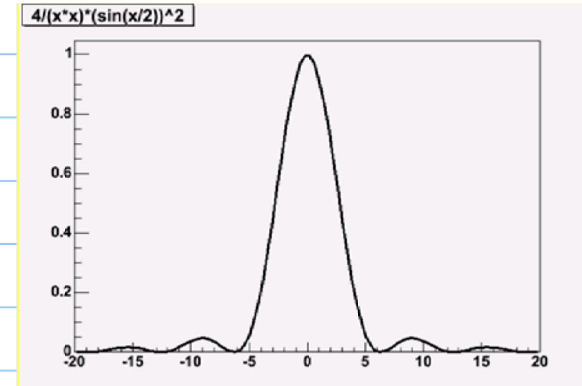
$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{3}{2a^3}} \left[\underbrace{\int_{-a}^{0} K\, e^{iKx}\, dK}_{①} - \underbrace{\int_{0}^{a} K\, e^{iKx}\, dK}_{②} + a \underbrace{\int_{-a}^{a} e^{iKx}\, dK}_{③} \right]$$

$$① = \frac{a}{ix} e^{-iax} + \frac{1}{x^2}\left(1 - e^{-ix}\right), \quad ② = \frac{a}{ix} e^{iax}\left(e^{ix} - 1\right)$$

$$③ = \frac{1}{ix}\left(e^{iax} - e^{-iax}\right) = \frac{2\sin(ax)}{x}$$

Example 2 continued:

$$(1)+(2)+(3) = \frac{4}{x^2}\sin^2\left(\frac{ax}{2}\right)$$



Example 3:

→ Find $\psi(x)$ if $A(k) = A \exp\left[-a^2(k-k_0)^2/4\right]$

First let's find A: $1 = \int_{-\infty}^{\infty} |A(k)|^2 dk$

$$= |A^2| \int_{-\infty}^{\infty} dk \exp\left[-\frac{a^2}{2}(k-k_0)^2\right]$$

with $z = k - k_0$, we have

$$\int_{-\infty}^{\infty} e^{-a^2 z^2/2}\, dz = \sqrt{\frac{2\pi}{a}}$$

$$\Rightarrow A = \left[a^2/2\pi\right]^{1/4}$$