Free particle

Note Title 9/21/2010

If $V(x)=0$ everywhere, T.I.S.E. reads

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

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

The general solution for this 2nd order diff eq. is $\psi(x)=Ae^{ikx}+Be^{-ikx}$.

Since there are not any boundary conditions, all values of "k" are possible.

With the standard time dependence of $e^{-i\frac{E}{\hbar}t}$, the time dependent separable solution becomes

$$\Psi(x,t)=\psi(x)\,e^{-i\frac{E}{\hbar}t}$$

$$=Ae^{ikx-i\frac{\hbar k^2}{2m}t}+Be^{-ikx-i\frac{\hbar k^2}{2m}t}$$

$$=Ae^{ik(x-\frac{\hbar k}{2m}t)}+Be^{-ik(x+\frac{\hbar k}{2m}t)}.$$

Here $e^{ik(x-\frac{\hbar k}{2m}t)}$ corresponds to a wave function propagating to the right and $e^{-ik(x+\frac{\hbar k}{2m}t)}$ corresponds to one to the left, with phase velocities of $\frac{\hbar k}{2m}$ & $-\frac{\hbar k}{2m}$ each.

Or if we allow "k" to take negative values as well such that $k=\pm\frac{\sqrt{2mE}}{\hbar}$,

$k>0 \Rightarrow$ traveling to the right

$k<0 \Rightarrow$ " " left,

with $v_{phase}=\frac{\hbar k}{2m}$

* For comparison, de Broglie formula provides

$$p = \hbar k \Rightarrow v = \frac{p}{m} = \frac{\hbar k}{m}$$

If we call this speed classical speed $v_{classical}$

$$v_{classical} = \frac{\hbar k}{m} = 2\, v_{phase}$$

(or $v_{quantum}$)

We will discuss this more later on.

* The free particle eigenfunction Ae^{ikx} is not normalizable because

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

So free particle state is not a stationary state. But it is still useful to describe scattering and tunneling problem later on.

* Still the most general wave function for a free particle is given by

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

$$" \frac{E_k}{\hbar}$$

Compare this with the discrete case such as the infinite well problem, where

$$\Psi(x,t) = \sum_{n=1,2\ldots}^{\infty} c_n \psi_n(x)\, e^{-i\frac{E_n}{\hbar}t}$$

Discrete		free particle (continuous)
n	$\Leftrightarrow$	k
C_n	$\Leftrightarrow$	$\frac{1}{\sqrt{2\pi}}\phi(k)$
$\psi_n(x)$	$\Leftrightarrow$	e^{ikx}
E_n	$\Leftrightarrow$	E_k

* The most general problem is : Given $\Psi(x,0)$ for $t=0$, Find $\Psi(x,t)$

$\boxed{\text{Answer:}}$ Use the Fourier and inverse Fourier transformation, which are

$$\boxed{\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk \\ \Leftrightarrow \quad F(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx \end{aligned}}$$

So

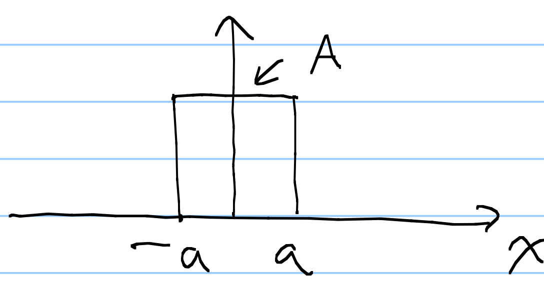
$$\underbrace{\Psi(x,0)}_{\text{Given}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underbrace{\phi(k)}_{\text{unknown}}\, e^{ikx}\, dx$$

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

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

$\boxed{\text{Ex.}}$ At $t=0$

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



$\Rightarrow$ Find $\Psi(x,t)$.

[Note; although the eigenfcns of T.I.S.E, $\psi(x)$ are always continuous, $\Psi(x,0)$ does not have to be as in this case]

Normalize first ; $|A|^2 \cdot 2a = 1 \Rightarrow A = \frac{1}{\sqrt{2a}}$

Now evaluate $\phi(k)$

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

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

$$\left[\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i} \right]$$

So

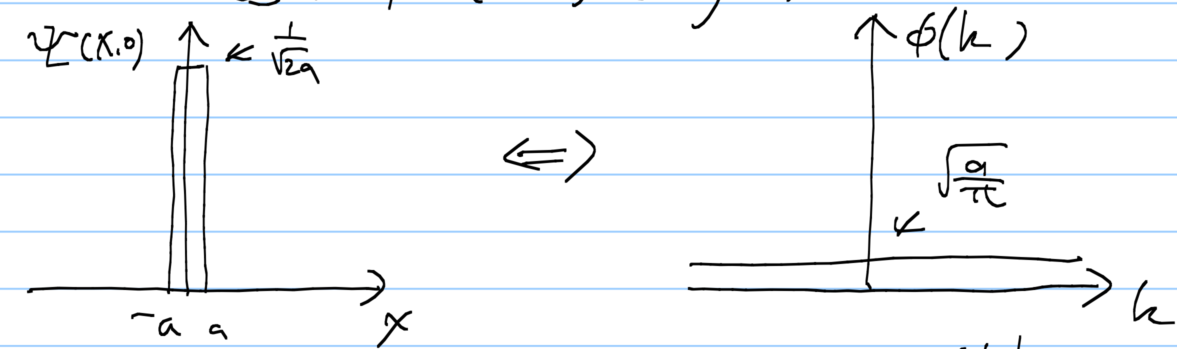
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx - \frac{\hbar k^2}{2m}t)} dk$$

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

In order to get a feeling on how this ftn behaves, if "a" is very small

$$\phi(k) = \frac{1}{\sqrt{\pi a}} \frac{\sin(ka)}{k} \approx \frac{1}{\sqrt{\pi a}} \frac{ka}{k} = \sqrt{\frac{a}{\pi}}$$

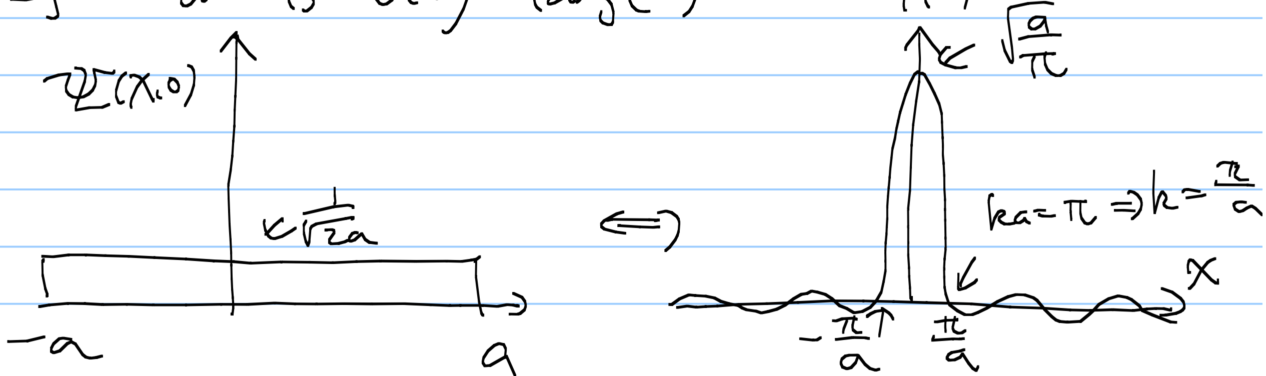
In other words, if "a" is very small



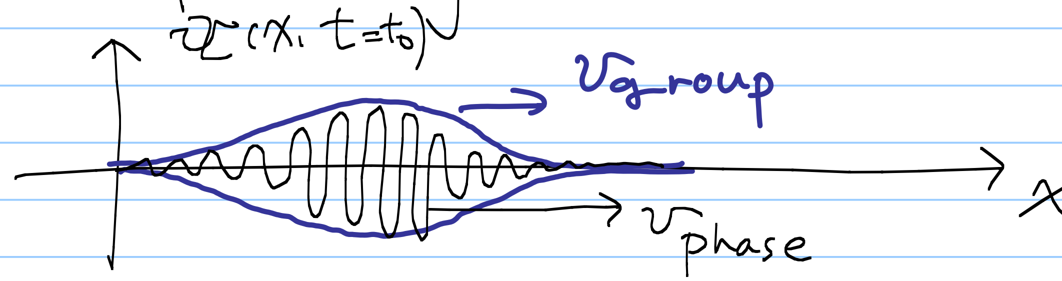
position well-defined ($x \approx 0$)

momentum ($\hbar k$) ill-defined

If "a" is very large,



* Group velocity vs. Phase velocity



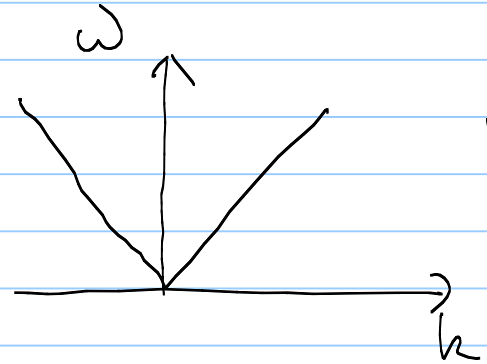
- For water waves $v_g = \frac{1}{2} v_p$
- For quantum mechanical wave fcns for a free particle satisfying Shrödinger Eq.

$$v_g = 2 v_p$$

- Generally, $v_g = \frac{d\omega}{dk}$ and $v_p = \frac{\omega}{k}$, where $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx-\omega t)} dk$ with $\omega \equiv \frac{E}{\hbar}$.

- $\omega \left(= \frac{E}{\hbar}\right)$ vs. $k \left(= \frac{p}{\hbar}\right)$ is called "dispersion relation"

$\boxed{\text{Ex.}}$ ① photon (electro magnetic wave)



$\omega = kc$
c: speed of light

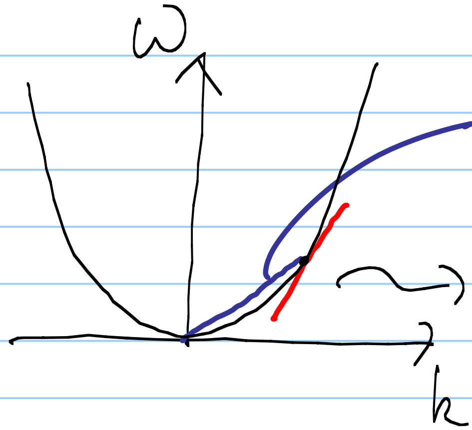
⌈Or equivalently $E = pc$⌋

For photon, $\underline{v_g} = \frac{d\omega}{dk} = c = \frac{\omega}{k} = \underline{v_p}$

② For a massive free particle,

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

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



$$\text{slope} = \frac{\omega}{k} = v_p = \frac{\hbar k}{2m}$$

$$\text{slope} = \frac{d\omega}{dk} = v_g = \frac{\hbar k}{m}$$

So $v_g = 2 v_p$

Note that

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

describes wave functions of any arbitrary particles, either massless or massive, in free space.