LECTURE #4

CONSIDER A FREE PARTICLE (i.e., $V(x)=0$)

CLASSICALLY, THE FREE PARTICLE TRAVELS AT A CONSTANT VELOCITY: $V_{CLASSICAL} = \sqrt{\frac{2E}{m}}$ (SINCE $E = \frac{1}{2}mv^2$)

QUANTUM MECHANICALLY, WE MUST SOLVE THE TIME-INDEPENDENT SCHRÖDINGER EQUATION:

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

OR $$\frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{WHERE } k = \frac{\sqrt{2mE}}{\hbar}$$

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

$$\Rightarrow \Psi(x,t) = Ae^{ikx}e^{-iEt/\hbar} + Be^{-ikx}e^{-iEt/\hbar}$$

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

$$\Psi(x,t) = \underbrace{Ae^{i(kx - \frac{\hbar k^2}{2m}t)}}_{\text{PROPAGATING WAVE TO THE RIGHT}} + \underbrace{Be^{-i(kx + \frac{\hbar k^2}{2m}t)}}_{\text{PROPAGATING WAVE TO THE LEFT}}$$

SINCE THESE TWO TERMS ONLY DIFFER IN THE SIGN OF K, IT IS MORE CONCISE TO WRITE:

$$\Psi_k(x,t) = Ae^{i(kx - \frac{\hbar k^2}{2m}t)} \quad \text{WHERE } k = \pm\frac{\sqrt{2mE}}{\hbar}$$

RIGHT

LEFT

THE STATIONARY STATES OF THE FREE PARTICLE ARE PROPAGATING WAVES WITH:

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

SINCE $p = \frac{h}{\lambda}$ (DE BROGLIE FORMULA), $p = \hbar k$

FURTHERMORE, THE SPEED OF THESE WAVES IS:
(COEFFICIENT OF t OVER THE COEFFICIENT OF x)

$$V_{QUANTUM} = \frac{\hbar |k|}{2m} = \sqrt{\frac{E}{2m}} = \frac{1}{2} V_{CLASSICAL}$$

THIS MYSTERIOUS FACTOR OF $\frac{1}{2}$ WILL BE ADDRESSED LATER.

MORE CONCERNING IS THE FACT THAT THIS WAVE FUNCTION IS NOT NORMALIZABLE:

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

$\Rightarrow$ A FREE PARTICLE CANNOT EXIST IN A STATIONARY STATE.

i.e., THERE IS NO SUCH THING AS A FREE PARTICLE WITH A DEFINITE ENERGY!

HOWEVER, WE SHOULD BE ABLE TO CONSTRUCT THE GENERAL SOLUTION FROM THE SEPARABLE SOLUTIONS.

SINCE k IS CONTINUOUS, THE GENERAL SOLUTION WILL BE AN INTEGRAL INSTEAD OF A SUM:

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

NOTE: $\frac{1}{\sqrt{2\pi}} \phi(k)\,dk$ PLAYS THE ROLE OF c_n

FOR APPROPRIATE $\phi(k)$, THIS WAVE FUNCTION CAN BE NORMALIZED. IT ALSO CONTAINS A RANGE OF K AND THUS A RANGE OF ENERGY AND SPEED.

→ "WAVE PACKET"

TYPICALLY, WE ARE GIVEN $\Psi(x,0)$ AND NEED TO FIND $\Psi(x,t)$.

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

STEP #2: FOURIER TRANSFORM TO FIND $\phi(k)$:

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

STEP #3: PLUG $\phi(k)$ INTO THE GENERAL SOLUTION:

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

EXAMPLE: A FREE PARTICLE INITIALLY LOCALIZED IN THE RANGE $-a < x < a$ IS RELEASED AT $t=0$.

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

FIRST NORMALIZE $\Psi(x,0)$ TO FIND A:

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

NEXT, CALCULATE $\phi(k)$:

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

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

FINALLY, PLUG $\phi(k)$ INTO THE GENERAL SOLUTION:

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

THIS INTEGRAL CANNOT BE SOLVED ANALYTICALLY BUT CAN BE EVALUATED NUMERICALLY → $\boxed{\text{FIG. 2.8}}$

ALSO CONSIDER LIMITING CASES:

(1) a IS SMALL $\Rightarrow \sin(ka) \simeq ka \Rightarrow \phi(k) = \sqrt{\frac{a}{\pi}}$

LOCALIZATION IN SPACE $\Rightarrow$ LARGE SPREAD IN $k = \frac{p}{\hbar}$

* CONSISTENT W/ UNCERTAINTY PRINCIPLE → $\boxed{\text{FIG. 2.9}}$

(2) a IS LARGE: SINCE $\frac{\sin(ka)}{ka}$ FIRST DROPS TO ZERO AT $k = \pm\pi/a$, $\phi(k)$ IS A SHARP SPIKE ABOUT $k=0$ → $\boxed{\text{FIG. 2.10}}$

FIG. 2.11 A WAVE PACKET IS A SUPERPOSITION OF SINUSOIDAL FUNCTIONS WHOSE AMPLITUDE IS MODULATED BY $\phi(k)$

i.e., IT CONTAINS RIPPLES WITHIN AN ENVELOPE

THE PARTICLE VELOCITY IS NOT THE SPEED OF THE INDIVIDUAL RIPPLES (PHASE VELOCITY) BUT RATHER THE SPEED OF THE ENVELOPE (GROUP VELOCITY)

EARLIER, WE CALCULATED $V_{QUANTUM} = \frac{1}{2} V_{CLASSICAL}$ BUT THIS WAS THE PHASE VELOCITY

HOWEVER, WHAT MATTERS IS THE GROUP VELOCITY:

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

WHERE, IN OUR CASE, $\omega = \frac{\hbar k^2}{2m}$ (DISPERSION RELATION)

ASSUME $\phi(k)$ IS PEAKED ABOUT k_0

$\Rightarrow$ TAYLOR SERIES EXPAND $\omega(k)$ ABOUT k_0:

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

NOTE: $\omega_0 = \omega(k_0)$, $\omega_0' = \left.\frac{d\omega}{dk}\right|_{k=k_0}$

CHANGE VARIABLES FROM k TO $s = k - k_0$,

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

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

FOR $t>0$,

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

EXCEPT FOR THE SHIFT FROM x TO $x-\omega_0' t$, THIS INTEGRAL IS THE SAME AS $\Psi(x,0)$

$$\therefore \quad \Psi(x,t) \simeq e^{-i(\omega_0 - k_0\omega_0')t}\, \Psi(x-\omega_0' t, 0)$$

PHASE FACTOR THAT DOESN'T AFFECT $|\Psi|^2$

$\therefore$ WAVE PACKET MOVES AT A SPEED ω_0'

i.e., $V_{GROUP} = \omega_0' = \left.\frac{d\omega}{dk}\right|_{k=k_0}$

SINCE $\omega = \frac{\hbar k^2}{2m}$, $\frac{d\omega}{dk} = \frac{\hbar k}{m} = \frac{p}{m} = V_{CLASSICAL}$

$\therefore$ QUANTUM MECHANICAL FREE PARTICLES TRAVEL AS WAVE PACKETS WITH A GROUP VELOCITY THAT FOLLOWS THE CLASSICAL EQUATIONS OF MOTION.

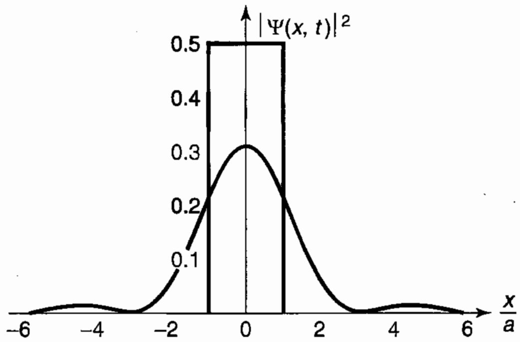

FIGURE 2.8: Graph of $|\Psi(x, t)|^2$ (Equation 2.104) at $t = 0$ (the rectangle) and at $t = ma^2/\hbar$ (the curve).

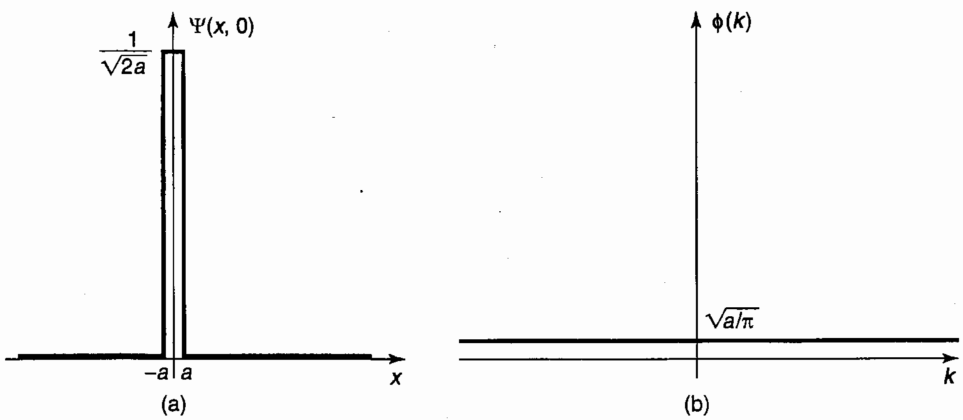

FIGURE 2.9: Example 2.6, for small a. (a) Graph of $\Psi(x, 0)$. (b) Graph of $\phi(k)$.

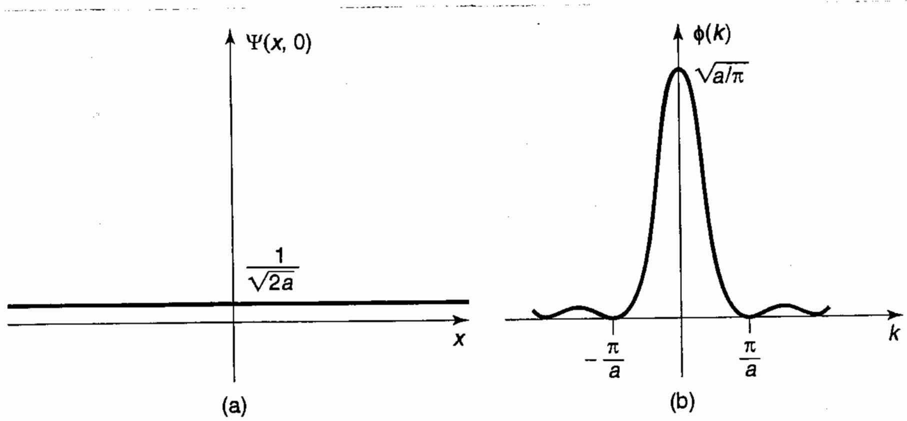

FIGURE 2.10: Example 2.6, for large a. (a) Graph of $\Psi(x, 0)$. (b) Graph of $\phi(k)$.

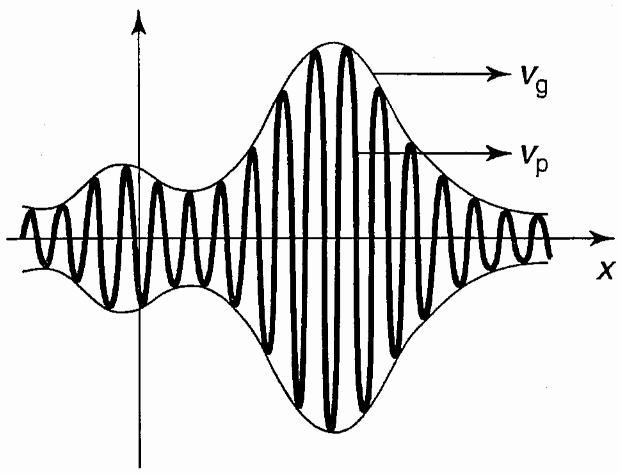

FIGURE 2.11: A wave packet. The "envelope" travels at the group velocity; the "ripples" travel at the phase velocity.