Physics 371 Lecture 8

Wave-packet dynamics and scattering in 1D

Consider the wave packet

$\Psi(x, t=0) = B e^{ik_0 x - \sigma_k^2 x^2}$, which was discussed in lecture 4.

How does it evolve with time?

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \quad \text{(free particle)}$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{\Psi}(k,t)\, e^{ikx}$$

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[i\hbar \frac{\partial \tilde{\Psi}(k,t)}{\partial t} - \frac{\hbar^2 k^2}{2m} \tilde{\Psi}(k,t) \right] e^{ikx} = 0$$

$$\Rightarrow \quad i\hbar \frac{\partial \tilde{\Psi}}{\partial t}(k,t) = \frac{\hbar^2 k^2}{2m} \tilde{\Psi}(k,t)$$

Solution:

$$\tilde{\Psi}(k,t) = \tilde{\Psi}(k, t=0)\, e^{-i\omega_k t}$$

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

$$\Psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, \tilde{\Psi}(k, t=0)\, e^{i(kx - \omega_k t)}$$

$$= A \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ikx - i\omega_k t - \frac{(k-k_0)^2}{4\sigma_k^2}}$$

Let us expand

- $$\omega_k = \omega_0 + \left.\frac{d\omega}{dk}\right|_{k_0}(k-k_0) + \frac{1}{2}\frac{d^2\omega}{dk^2}(k-k_0)^2 + \dots$$

$$\omega_0 = \frac{\hbar k_0^2}{2m} \qquad \left.\frac{d\omega}{dk}\right|_{k_0} = \frac{\hbar k_0}{m} = v_g$$

group velocity

= particle speed

- $$\left.\frac{d^2\omega}{dk^2}\right|_{k_0} = \frac{\hbar}{m}$$

$$\omega_k \simeq \omega_0 + v_g(k-k_0) + \frac{\hbar}{2m}(k-k_0)^2$$

$$\Psi(x,t) = A e^{i(k_0 x - \omega_0 t)} \int_{-\infty}^{\infty} \frac{dk}{2\pi}$$

- $$\times\, e^{i(k-k_0)(x-v_g t) - a(k-k_0)^2}$$

- $$a = \frac{1}{4\sigma_k^2} + \frac{i\hbar t}{2m}$$

Completing the square, and performing the Gaussian integral, one finds

- $$\Psi(x,t) = C\, e^{i(k_0 x - \omega_0 t) - \frac{(x - v_g t)^2}{4a}}$$

Phase velocity $\quad v_p = \frac{\omega_0}{k_0} = \frac{\hbar k_0}{2m}$

$$= \frac{1}{2} v_g$$

$$\rho(x,t) = C^2 e^{-(x - v_g t)^2 \left(\frac{1}{4a} + \frac{1}{4a^*}\right)}$$

$$= C^2 e^{-\frac{(x - v_g t)^2}{2\sigma_x(t)^2}}$$

$\rightarrow$ probability wave packet moves at v_g

- $$\sigma_x(t) = \frac{1}{2\sigma_k}\sqrt{1 + \left(\frac{2\hbar\sigma_k^2}{m} t\right)^2}$$

- For long times,

$$\sigma_x(t) \simeq \frac{\hbar \sigma_k}{m} t = \frac{\hbar \Delta k}{m} t$$

$$= \Delta v \, t .$$

$$\Delta x \, \Delta p_x = \frac{\hbar}{2} \sqrt{1 + \left(\frac{2\hbar \sigma_k^2 t}{m}\right)^2} \geq \frac{\hbar}{2}$$

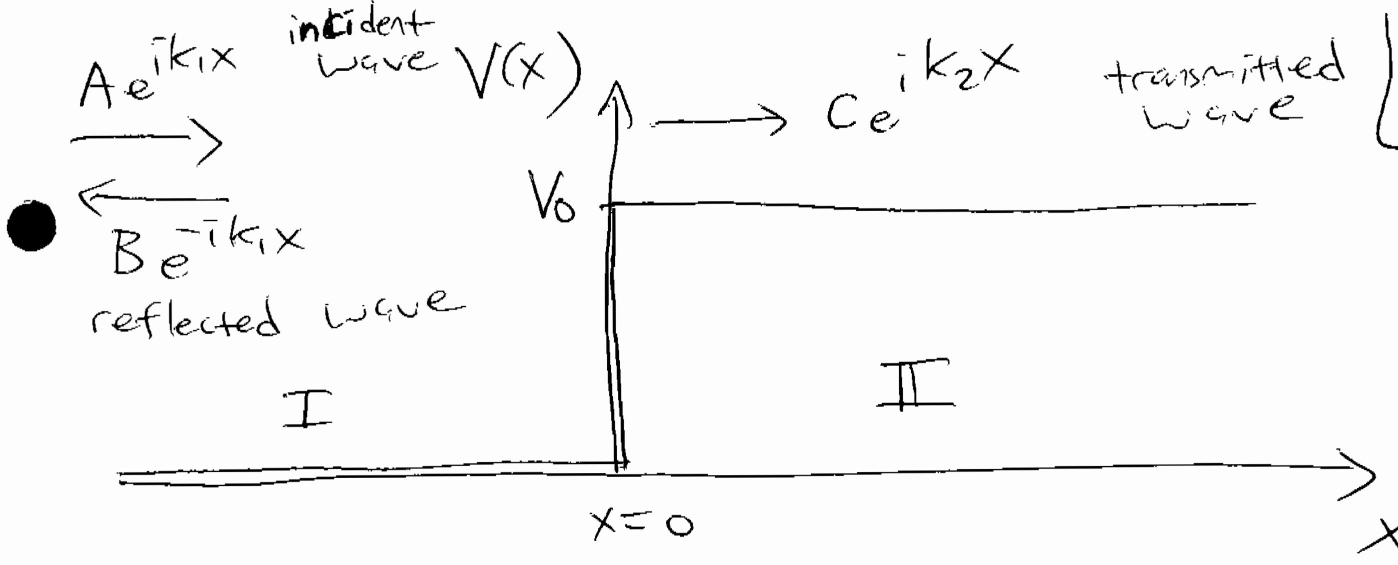
minimum-uncertainty wavepacket spreads in coordinate space, retains shape in momentum space. Product of uncertainties increases with time.

1D Scattering

Scattering involves shooting a wavepacket at a target, and observing the outgoing particle(s).

As we have seen, a wave packet can be built from a linear superposition of plane waves, and the dynamics of a plane wave is much simpler. By choosing the appropriate boundary conditions, we can study scattering with plane waves.

As the simplest example, consider scattering from a potential step:



Region I: $E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$

Region II: $(E-V_0)\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$

$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$,

$\psi_{II}(x) = Ce^{ik_2x}$ solve Sch. eq.

in regions I and II separately,

provided $E = \frac{\hbar^2 k_1^2}{2m}$,

$E = \frac{\hbar^2 k_2^2}{2m} + V_0$.

(assuming $E > V_0$)

The coefficient A is determined by the incident probability current:

$$j_{in} = \frac{1}{2m}\left(\psi_{in}^{*} \frac{\hbar}{i} \frac{d\psi_{in}}{dx} - \psi_{in} \frac{\hbar}{i} \frac{d\psi_{in}^{*}}{dx}\right)$$

$$\psi_{in}(x) = A e^{ik_1 x}$$

$$j_{in} = \frac{\hbar k_1}{m} |A|^2.$$

How do we determine the coefficients B & C?

i) The wavefunction must be continuous at $x=0$, otherwise the momentum would blow up:

$$\psi_{I}(0) = \psi_{II}(0)$$

iii) The first derivative of ψ must be continuous at $x=0$, otherwise the kinetic energy would blow up:

$$\psi_{I}'(0) = \psi_{II}'(0).$$

i) $A + B = C$

ii) $ik_1(A-B) = ik_2 C$

$$\Rightarrow \quad A - B = \frac{k_2}{k_1} C$$

$$2A = \left(1 + \frac{k_2}{k_1}\right) C$$

$$\Rightarrow \quad C = \frac{2k_1}{k_1+k_2} A$$

$$B = C - A = \frac{k_1 - k_2}{k_1 + k_2} A$$

Current conservation:

$$j_{in} = \frac{\hbar k_1}{m} |A|^2$$ incident current

$$j_{tr} = \frac{\hbar k_2}{m} |C|^2$$ transmitted "

$$j_{re} = -\frac{\hbar k_1}{m} |B|^2$$ reflected "

Let $R = \frac{|j_{re}|}{|j_{in}|}$ = reflection probability

and $T = \left| \frac{j_{tr}}{j_{in}} \right|$ = transmission probability

- $$R = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

$$T = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2} = \frac{4 k_1 k_2}{(k_1 + k_2)^2}$$

$$R + T = 1$$

- Note that R is independent of the sign of the potential step; a step down is equally effective at reflecting the wavepacket as a step up. Note that a classical particle with $E > V_0$ would <u>not</u> be reflected by the step.

<u>Q: what if $E < V_0$?</u>

$$\psi_I(x) = A e^{ik_1 x} + B e^{-ik_1 x}$$

$$\psi_{II}(x) = C e^{-K_2 x},$$

$$K_2 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

(exponentially growing solution is not normalizable).

i) $A + B = C$

ii) $ik_1(A - B) = -K_2 C$

$$A - B = i\frac{K_2}{k_1} C$$

$$C = \frac{2k_1}{k_1 + iK_2} A$$

$$B = \frac{k_1 - iK_2}{k_1 + iK_2} A$$

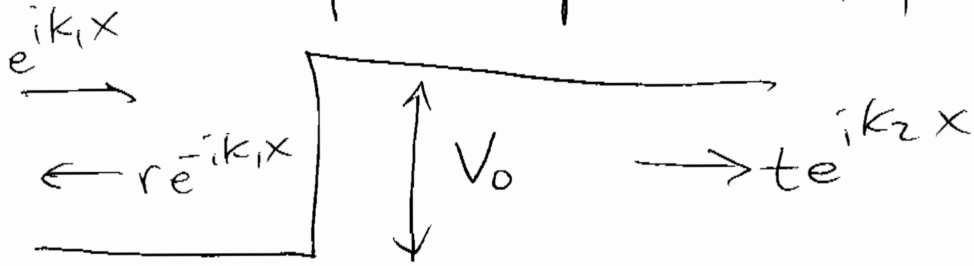
Since ψ_{II} is real,

$$j_{tr} = 0$$

$$T = 0, \quad R = \left|\frac{B}{A}\right|^2 = \underline{1}$$

All particles are reflected, as in the classical case.

Step potential



$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

$$E = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2 k_2^2}{2m} + V_0$$

$$k_1^2 = k_2^2 + \frac{2mV_0}{\hbar^2}$$

let $\dfrac{2mV_0}{\hbar^2} = k_0^2$, $x = \dfrac{k_1}{k_0}$

$$k_2^2 = k_1^2 - k_0^2$$

$$R^{1/2} = \frac{k_1 - \sqrt{k_1^2 - k_0^2}}{k_1 + \sqrt{k_1^2 - k_0^2}} = \frac{\left(k_1 - \sqrt{k_1^2 - k_0^2}\right)^2}{k_0^2}$$

$$R = \left(x - \sqrt{x^2 - 1}\right)^4 , \quad T = 1 - R$$