PHY202 – Quantum Mechanics
Summary of Topic 9: Quantum propagation

Wavepacket propagation

Recall

- a wavepacket consisting of a continuous spectrum of momenta p

  (e.g., unbound (free) states, or bound states in x-dependent potential $V(x)$)

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp\, \phi(p) \exp\left(\frac{i}{\hbar}px\right)$$

  $\phi(p)$ – (in general complex) momentum profile

- the full time dependent wavefunction is given by

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp\, \phi(p) \exp\left(\frac{i}{\hbar}px\right) \exp\left(-\frac{i}{\hbar}Et\right)$$

  where $E = p^2/2m + V(x)$ is the total energy

- Time evolution of $\Psi(x,t)$ is in general very complicated, even for fairly simple cases like Gaussian profiles.

Below we will consider some simplified cases. First let's introduce some useful and general language.

Quantum mechanical current

- Recall, the probability density is given by

$$P(x,t) = |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$$

- introduce a probability current $j(x,t)$ (also called probability flux)

$$\boxed{j(x,t) = -i\frac{\hbar}{2m}\left[\Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x} - \Psi(x,t)\frac{\partial\Psi^*(x,t)}{\partial x}\right]}$$

  Sign convention: $j(x,t) > 0$ (< 0) means flux moving right (left).

- if $\Psi(x,t)$ is a solution of the TDSE, then $P(x,t)$ and $j(x,t)$ satisfy a continuity equation

$$\boxed{\frac{\partial P(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x}}$$

- Physical interpretation: conservation of probability.
  The change of the probability density at x is equal to its "outflow" from there.

- Analogous to: electric charge current, gas density and flow, etc.

Examples

- take a stationary state $\Psi(x,t) = \psi(x) \exp\left(-\frac{i}{\hbar}Et\right)$, with $\psi(x)$ satisfying the TISE and total energy E. Then

$$\boxed{j(x,t) = -i\frac{\hbar}{2m}\left[\psi^*(x)\frac{\partial\psi(x)}{\partial x} - \psi(x)\frac{\partial\psi^*(x)}{\partial x}\right]}$$

  Note $j(x)$ is independent of time! Interpretation: constant flux.

- take $\psi(x)$ to be a momentum eigenfunction $\psi_p(x) = \exp\left(\frac{i}{\hbar}px\right)$,

$$\boxed{j(x,t) = -i\frac{\hbar}{2m}\left[\psi^*(x)\frac{\partial\psi(x)}{\partial x} - \psi(x)\frac{\partial\psi^*(x)}{\partial x}\right] = \frac{p}{m}}$$

  Interpretation: classically $\frac{p}{m} = v$ is velocity.

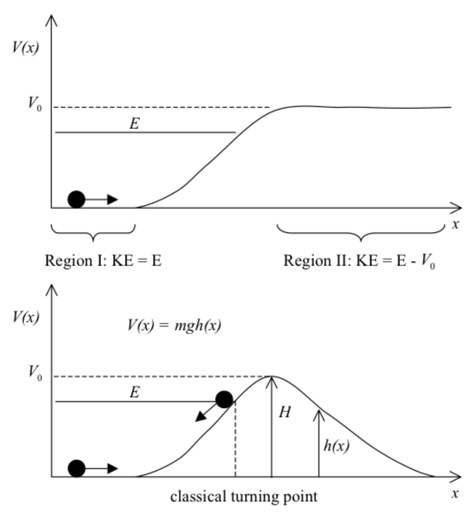
- take $\psi(x)$ to be a real function (like in bound states)

$$\boxed{j(x,t) = 0}$$

  Interpretation: a bound state of definite energy is a standing wave.

Classical Potential Steps and Barriers

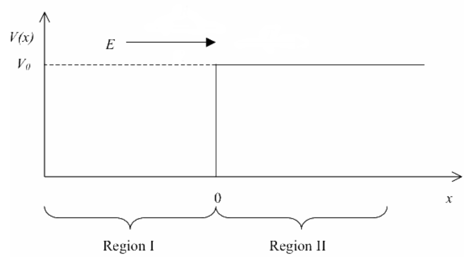
Consider a flux of particles incident from the left on the potential step or barrier.



- if $E > V_0$, all the particles will pass over the step/barrier (they are transmitted)
- they will slow down (smaller momentum)
- if $E < V_0$, all the particles are reflected
- In both cases the flux of particles must be the same. (They don't sink anywhere.)

Quantum mechanical potential step $E > V_0$

Consider a flux of particles with total energy E incident from the left on a square potential step. Assume $E > V_0$.



- $x < 0$ (Region I):

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$
$$\Rightarrow \psi''(x) = -k_1^2\psi(x) \quad k_1^2 = \frac{2mE}{\hbar^2} > 0$$

The physical solutions are

KE: $T_1 = \frac{\hbar^2 k_1^2}{2m} = E$

$$\boxed{\psi_I(x) = \underbrace{A\exp(ik_1x)}_{\text{incident}} + \underbrace{R\exp(-ik_1x)}_{\text{reflected}}}$$

A, R – (complex) amplitudes

- $x \geq 0$ (Region II):

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\psi(x) = E\psi(x)$$
$$\Rightarrow \psi''(x) = -k_2^2\psi(x) \quad k_2^2 = \frac{2m(E-V_0)}{\hbar^2} > 0 \qquad k_2 < k_1$$

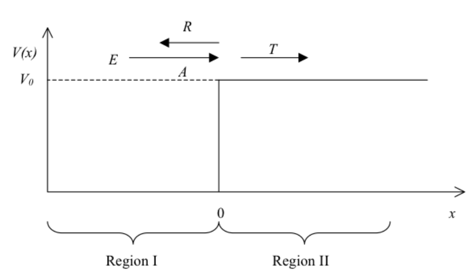
The physical solution is

KE: $T_2 = \frac{\hbar^2 k_2^2}{2m} = E - V_0 > 0$

$$\boxed{\psi_{II}(x) = \underbrace{T\exp(ik_2x)}_{\text{transmitted}}}$$

T – (complex) amplitude

Reflection and transmission



Compute the currents:

- $x < 0$

$$\begin{aligned} j_I &= |A|^2\frac{p_1}{m} &= |A|^2\frac{k_1\hbar}{m} \quad &\text{incident beam} \\ j_R &= -|R|^2\frac{p_1}{m} &= -|R|^2\frac{k_1\hbar}{m} \quad &\text{reflected beam} \end{aligned}$$

Note that $j_I > 0$ but $j_R < 0$

- $x \geq 0$

$$j_T \quad = \quad |T|^2 \frac{p_2}{m} \quad = \quad |T|^2 \frac{k_2 \hbar}{m} \qquad \text{transmitted beam}$$

Introduce:

- the probability of reflection P_R

$$P_R = \frac{|j_R|}{|j_I|} = \frac{|R|^2 k_1 \hbar/m}{|A|^2 k_1 \hbar/m} = \frac{|R|^2}{|A|^2} = |\frac{R}{A}|^2$$

- the probability of transmission P_T

$$P_T = \frac{|j_T|}{|j_I|} = \frac{|T|^2 k_2 \hbar/m}{|A|^2 k_1 \hbar/m} = \frac{|T|^2}{|A|^2} \frac{k_2}{k_1} = |\frac{T}{A}|^2 \frac{k_2}{k_1}$$

Apply boundary conditions on the wavefunction at $x = 0$:

$$\begin{array}{lll} \psi_I(x=0) = \psi_{II}(x=0) & \Rightarrow & A + R = T \\ \psi'_I(x=0) = \psi'_{II}(x=0) & \Rightarrow & ik_1(A - R) = ik_2 T \end{array}$$

Eliminate T:

$$\frac{R}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$

Eliminate R:

$$\frac{T}{A} = \frac{2k_1}{k_1 + k_2}$$

This leads to:

$$\begin{array}{lllll} P_R & = & |\frac{R}{A}|^2 & = & \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \\ P_T & = & |\frac{T}{A}|^2 \frac{k_2}{k_1} & = & \frac{4 k_1 k_2}{(k_1 + k_2)^2} \end{array}$$

Note: $\boxed{P_R + P_T = 1}$

This is a reflection of the fact that the current is conserved, $\boxed{j_I + j_R = j_T}$

(proof)

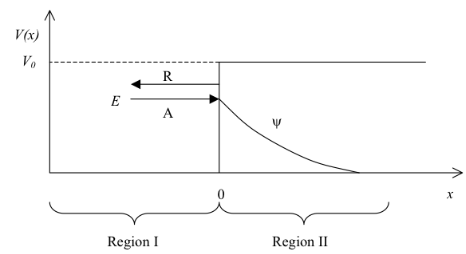
Comments:

- in the limit of a vanishing step, $V_0 \searrow 0$ or large energy, $E \gg V_0$:

$$k_2 \nearrow k_1 \quad \Rightarrow \quad P_R \searrow 0 \quad P_T \nearrow 1$$

Quantum mechanical potential step $E < V_0$

Consider a flux of particles with total energy E incident from the left on a square potential step. Assume now $E < V_0$.



- $x < 0$ (Region I): $k_1^2 = \frac{2mE}{\hbar^2} > 0$

  The solutions are the same as for $E > V_0$,

$$\boxed{\psi_I(x) = \underbrace{A\exp(ik_1x)}_{\text{incident}} + \underbrace{R\exp(-ik_1x)}_{\text{reflected}}}$$

- $x \geq 0$ (Region II):

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

$$\Rightarrow \psi''(x) = \alpha^2\psi(x) \quad \alpha^2 = \frac{2m(V_0-E)}{\hbar^2} > 0$$

  The solution is

  KE: $T_2 = E - V_0 < 0$!

$$\boxed{\psi_{II}(x) = \underbrace{T\exp(-\alpha x)}_{\text{tunnelling}}}$$

- the wavef'n $\psi_{II}(x)$ is real $\Rightarrow$ the current $j_T = 0$

$$\Rightarrow \text{ the probability of transmission } P_T = 0 \Rightarrow P_R = 1 - P_T = 1$$

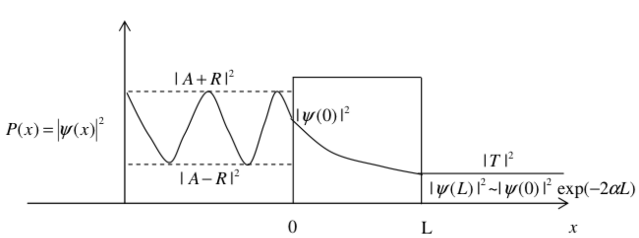
$$\boxed{\text{The whole beam is reflected.}}$$

as expected

- the penetration (tunneling) depth is $1/\alpha = \frac{\hbar}{\sqrt{2m(V_0-E)}}$

Tunnelling through a barrier

- If the step has a finite length L



- particle tunnelling between classically allowed regions can take place

$$P_T \simeq |\psi(L)|^2 \simeq |\psi(L)|^2 \exp(-2\alpha L)$$

$$\alpha^2 = \frac{2m(V_0-E)}{\hbar^2} > 0$$

See also http://yepes.rice.edu/PhysicsApplets/WavePacket.html

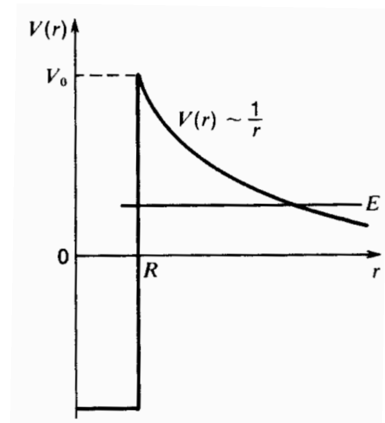
- The HUP for time and energy:

  let ΔE denote the uncertainty in the energy of the particle as it tunnels through the barrier and Δt the time needed to pass through it. Then

$$\boxed{\Delta E \Delta t \geq \frac{\hbar}{2}}$$

- during tunnelling the conservation of energy is violated but the HUP prevents us from observing it experimentally

Tunnelling in nature - examples



- α-decay of heavy nuclei

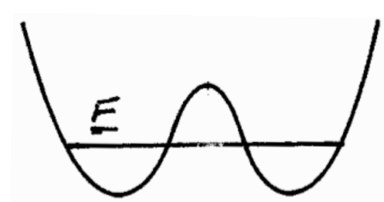
  α particles (^{4}He) tunnel through a nuclear potential barrier arising from the Coulomb repulsion

- nuclear fusion of light nuclei

  Nuclear fusion is essentially the inverse of -decay. Here light nuclei tunnel through the Coulomb barrier to form a strongly bound state. Quantum mechanical tunnelling is necessary to explain nuclear fusion in stars.

- covalent bonding

  Chemical bonding occurs via the tunnelling of electrons between nuclei. The electrons "resonate" between nuclei, thus lowering their energy and forming a bond.



Further reading:
See, e.g., Phillips, pages 94-103, 388-393.