

## Probability current and beams of particles

Let us consider the probability density  $P(x,t) = |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$ . So far we have encountered many cases where it is time independent i.e. it represents a stationary state, but what about the general case?

In general we can consider the rate of change of probability density, namely:

$$\frac{\partial P(x,t)}{\partial t}$$

where we do not expect it to be zero.

Let us consider an example of the time independent eigenstate yielding a constant probability density:

$$\Psi(x,t) = \psi_n(x)e^{-\frac{iE_nt}{\hbar}} \text{ results in } |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t) = |\psi_n(x)|^2 \text{ with } \frac{\partial P(x,t)}{\partial t} = 0$$

This is in contrast to a linear combination of such states, for example the state:

$$\Psi(x,t) = \frac{1}{\sqrt{2}} \left( \psi_1(x)e^{-\frac{iE_1t}{\hbar}} + \psi_2(x)e^{-\frac{iE_2t}{\hbar}} \right) \text{ where, using } |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$$

$$\text{we get } |\Psi(x,t)|^2 = |\psi_1|^2 + |\psi_2|^2 + 2 \operatorname{Re}\{\Psi_1^*(x,t)\Psi_2(x,t)\}$$

$$\text{or more simply } |\Psi(x,t)|^2 = |\psi_1|^2 + |\psi_2|^2 + 2\psi_1(x)\psi_2(x)\cos(\omega_{1-2}t) \text{ where } \omega_{1-2} = \frac{E_2 - E_1}{\hbar}$$

$$\text{this results in the clearly non-zero } \frac{\partial P(x,t)}{\partial t} = 2\omega_{1-2} \operatorname{Im}\{\Psi_1^*(x,t)\Psi_2(x,t)\} \neq 0$$

The general form of the rate of change of probability density is given by:

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial(\Psi^*(x,t)\Psi(x,t))}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi$$

the quantities  $\frac{\partial \Psi}{\partial t}$  and  $\frac{\partial \Psi^*}{\partial t}$  can be rewritten using the TDSE:

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi \text{ implies } \frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V\Psi \text{ and } \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V\Psi^*$$

substituting into the definition for the rate of change of probability density gives:

$$\frac{\partial P(x,t)}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi = \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left\{ \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right\}$$

The rate of change of probability density,  $\frac{\partial P(x,t)}{\partial t}$ , is related to the probability current,  $j(x,t)$ , by the simple relation:

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

so that the current itself is simply:

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

by taking into account the momentum operator,  $\hat{P} = -i\hbar \frac{\partial}{\partial x}$ , the current is rewritten

as:

$$j(x,t) = \frac{1}{2m} \{ \Psi^* \hat{P} \Psi - \Psi \hat{P} \Psi^* \} = \frac{1}{m} \text{Re} [\Psi^* \hat{P} \Psi]$$

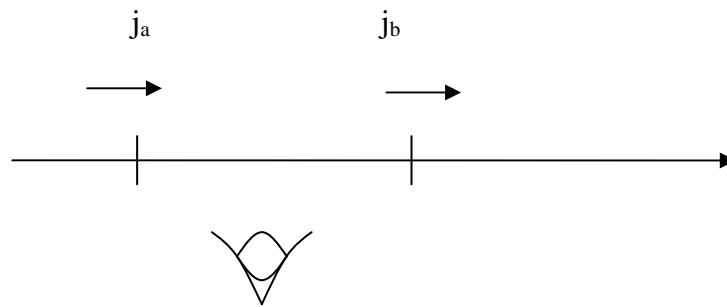
For a De Broglie matter wave we have:  $\Psi(x,t) = A e^{\frac{i}{\hbar}(P_x - Et)}$  and so the current becomes:

$$j(x,t) = \frac{P}{m} |A|^2 = v |A|^2 = \frac{\hbar k}{m} |A|^2$$

where  $A$  represents a number density (not a normalisation constant as the De Broglie matter wave is not normalisable).

To summarise:

The rate of change of probability density is equal to minus the current gradient



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

The current is given by:

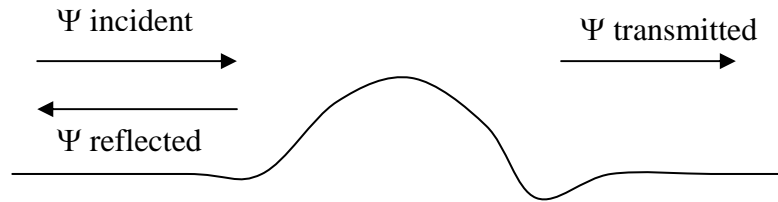
$$j(x,t) = \frac{1}{m} \text{Re} [\Psi^* \hat{P} \Psi]$$

and for a De Broglie wave it is simply:

$$j(x,t) = \frac{P}{m} |A|^2 = v |A|^2 = \frac{\hbar k}{m} |A|^2$$

## Reflection and Transmission – Scattering

Consider a beam incident from the left to the right towards the potential barrier shown:



Conservation of particles dictates:

$$j_{incident} = |j_{reflected}| + j_{transmitted}$$

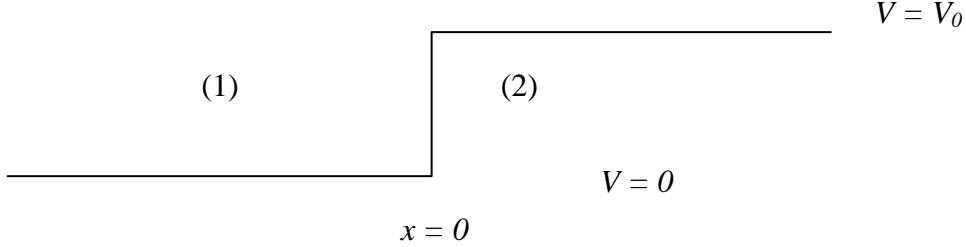
We can also define the reflection ( $R$ ) and transmission ( $T$ ) coefficients as:

$$R = \left| \frac{j_{ref}}{j_{inc}} \right| \quad \text{and} \quad T = \left| \frac{j_{trans}}{j_{inc}} \right|$$

Of course,  $R + T = 1 \dots$

## The potential step

Consider a beam of particles incident from the left on the potential step shown below:



Case I:  $E > V_0$

Region 1,  $V = 0$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + 0 = E\psi(x) \text{ becomes}$$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2} \psi(x) = -k^2 \psi(x) \text{ where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

giving the solutions:

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

which are identified as the incident and reflected waves...

Region 2,  $V = V_0$

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

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m(E - V_0)}{\hbar^2} \psi(x) = -q^2 \psi(x) \text{ where } q = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

giving solutions:

$$\psi(x) = Ce^{iqx} + De^{-iqx}$$

which we reduce to:  $\psi(x) = Ce^{iqx}$  since there is no source to the right of the step

We can write the probability flux as:

$$j_{inc} = |A|^2 \frac{\hbar k}{m}, \quad j_{ref} = |B|^2 \frac{\hbar k}{m} \quad \text{and} \quad j_{trans} = |C|^2 \frac{\hbar q}{m}$$

resulting in

$$R = \left| \frac{j_{ref}}{j_{inc}} \right| = \left| \frac{B}{A} \right|^2 \quad \text{and} \quad T = \left| \frac{j_{trans}}{j_{inc}} \right| = \frac{q}{k} \left| \frac{C}{A} \right|^2$$

We can now derive analytical expressions for these by applying boundary conditions at  $x = 0$

$$\psi \text{ continuous gives: } A + B = C \Rightarrow 1 + \frac{B}{A} = \frac{C}{A}$$

and  $\frac{d\psi}{dx}$  continuous gives:  $kA - kB = qC \Rightarrow 1 - \frac{B}{A} = \frac{q}{k} \frac{C}{A}$

which together yield  $\frac{C}{A} = \frac{2k}{k+q}$  and therefore  $T = \frac{4qk}{(k+q)^2}$  and  $R = \left(\frac{k-q}{k+q}\right)^2$

CASE II:  $E < V_0$

Region 1,  $V = 0$

Same as before, namely  $\psi(x) = Ae^{ikx} + Be^{-ikx}$

Region 2,  $V = V_0$

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

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m(V_0 - E)}{\hbar^2}\psi(x) = \kappa^2\psi(x) \text{ where } \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

giving solutions:

$\psi(x) = Ce^{-\kappa x} + De^{\kappa x}$  (decaying and rising exponentials)

which we reduce to:  $\psi(x) = Ce^{-\kappa x}$  since the wavefunction must tend to zero at infinity.

Let us now consider the probability density in the two regions.

In region 1 we have:

$\psi(x) = Ae^{ikx} + Be^{-ikx}$  and therefore  $|\psi|^2 = \psi^*\psi = A^2 + B^2 + 2AB \cos 2kx$

and in region 2:

$\psi(x) = Ce^{-\kappa x}$  and therefore  $|\psi|^2 = \psi^*\psi = |C|^2 e^{-2\kappa x}$

That is a stationary wave pattern in region 1 due to the interference of the incident and reflected particles and an evanescent decay in the classically forbidden region 2.