QUANTUM MECHANICS A (SPA-5319)

Probability Currents

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. where it represents a stationary state, but what about the general case? In general we can consider the rate of change of probability density, which we do not expect to be zero:

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

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

$$\Psi(x,t) = \psi_n(x) e^{-\frac{iE_n t}{\hbar}}$$

results in

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

with

$$\frac{\partial P(x,t)}{\partial t} = 0\,.$$

This is in contrast to what happens for a linear combination of such states. For example, consider the state:

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_1(x) e^{-\frac{iE_1 t}{\hbar}} + \psi_2(x) e^{-\frac{iE_2 t}{\hbar}}\right)$$

where, using $|\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$, we get

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

or, more simply,

$$|\Psi(x,t)|^2 = |\psi_1|^2 + |\psi_2|^2 + 2\psi_1(x)\psi_2(x)\cos(\omega_{1-2} t)$$

where $\omega_{1-2} = (E_2 - E_1)/\hbar$. This results in the following expression:

$$\frac{\partial P(x,t)}{\partial t} = 2\omega_{1-2}\,\mathrm{Im}\{\Psi_1^*(x,t)\Psi_2(x,t)\}$$

which is in general non-zero.

More generally, the form of the rate of change of probability density is given by

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

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

$$\frac{\partial\Psi}{\partial t}=\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2}-\frac{i}{\hbar}V\Psi \qquad \text{and} \qquad \frac{\partial\Psi^*}{\partial t}=-\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2}+\frac{i}{\hbar}V\Psi^*\,.$$

Substituting these into the definition for the rate of change of probability density gives:

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

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

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

where the current itself is simply given by

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

By using the momentum operator, $\hat{p}=-i\hbar\frac{\partial}{\partial x}$, this current can be rewritten as

$$j(x,t)=\frac{1}{2m}\left\{\Psi^*\hat{p}\Psi-\Psi\hat{p}\Psi^*\right\}=\frac{1}{m}\mathrm{Re}\left[\Psi^*\hat{p}\Psi\right]$$

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

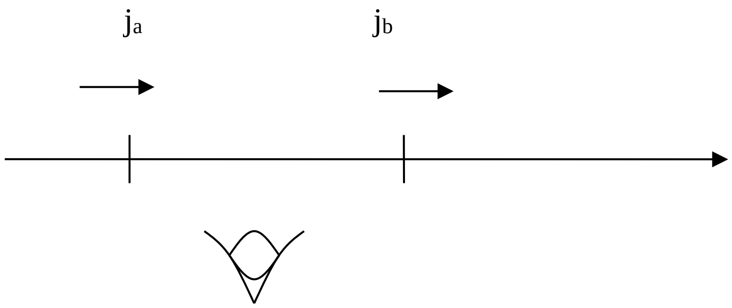
$$j(x,t)=\frac{p}{m}|A|^2=v|A|^2=\frac{\hbar k}{m}|A|^2$$

where *A* represents a number density (not a normalisation constant in this case, as the de Broglie matter wave is not normalisable).

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

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

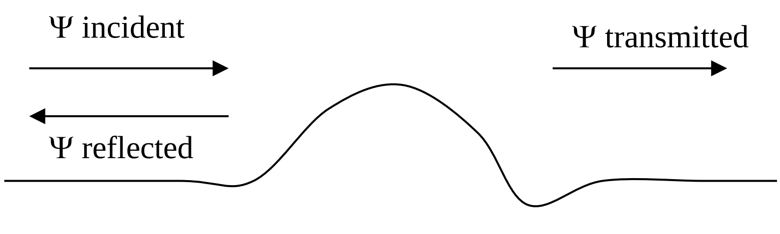
The current itself can be thought of as the amount of probability passing a given point:



The probability current is given by $j(x,t) = \frac{1}{m}\mathrm{Re}\left[\Psi^{*}\hat{P}\Psi\right]$, and for a de Broglie wave with $\Psi(x,t) = Ae^{\frac{i}{\hbar}(Px-Et)}$ 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 below:



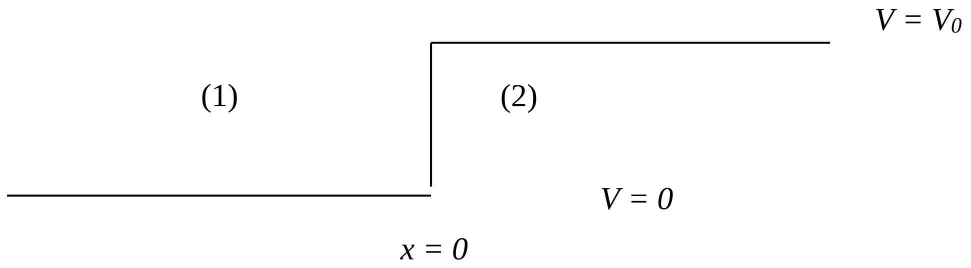
Conservation of particles dictates: $j_{incident} = \left|j_{reflected}\right| + j_{transmitted}$. We can also define the reflection (R) and transmission (T) coefficients as:

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

Of course, $R + T = 1$, due to the conservation of probability.

The potential step

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



Case I: *E* > *V₀*

In region 1, *V = 0* and $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+0=E\psi(x)$ becomes

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

This gives the solutions:

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

which can be identified as the incident and reflected waves.

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

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

This gives the solutions:

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

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

We can therefore write the probability currents as:

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

which result in

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

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

ψ being continuous gives: $\qquad A + B = C \Rightarrow 1 + \frac{B}{A} = \frac{C}{A}$

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

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 < V₀*

In region 1, *V = 0,* which is the same as before, namely $\psi(x) = Ae^{ikx} + Be^{-ikx}$.

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

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

giving solutions: $\psi(x) = Ce^{-\kappa x} + De^{\kappa x}$ (decaying and rising exponentials), which reduces to $\psi(x) = Ce^{-\kappa x}$ (as 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 $|\psi|^2 = \psi^*\psi = A^2 + B^2 + 2AB\cos 2kx$. In region 2 we have $\psi(x) = Ce^{-\kappa x}$, and therefore $|\psi|^2 = \psi^*\psi = |C|^2 e^{-2\kappa x}$.

That corresponds to 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.