QM I
Phys 651

Lecture #19

Interpretations of the wave function

We are familiar with the probability density

$$\rho(\vec{x},t) = |\Psi(\vec{x},t)|^2 = |\langle \vec{x}|\alpha, t_0; t\rangle|^2$$

$\Downarrow$

Introduce the probability flux $\Rightarrow$

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

$$\underset{\uparrow}{=} -\frac{i\hbar}{2m}\cdot 2i\,\mathrm{Im}(\Psi^*\vec{\nabla}\Psi) = \frac{\hbar}{m}\mathrm{Im}(\Psi^*\vec{\nabla}\Psi)$$

$a+ib-(a-ib) = 2ib$

Is there a connection between ρ and $\vec{j}$? $\Rightarrow$

$$\frac{\partial\rho}{\partial t} = \frac{\partial}{\partial t}(\Psi^*\Psi) = \underbrace{\frac{\partial\Psi^*}{\partial t}}_{=\frac{i}{\hbar}H\Psi^*}\Psi + \Psi^*\underbrace{\frac{\partial\Psi}{\partial t}}_{=-\frac{i}{\hbar}H\Psi} = \frac{i}{\hbar}\left((H\Psi^*)\Psi - \Psi^*(H\Psi)\right) =$$

$$= \frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}(\Delta\Psi^*)\Psi + \cancel{(V\Psi^*)\Psi} + \Psi^*\frac{\hbar^2}{2m}(\Delta\Psi) - \cancel{\Psi^*(V\Psi)}\right.$$

$$= \frac{i}{\hbar} \cdot \frac{\hbar^2}{2m} \left(\Psi^* \Delta \Psi - \Psi \Delta \Psi^* \right) = \frac{i\hbar}{2m} \cdot 2i \, \mathrm{Im} \left(\Psi^* \Delta \Psi \right)$$

$$= -\frac{\hbar}{m} \mathrm{Im} \left(\Psi^* \Delta \Psi \right)$$

Go back to $\vec{j}(\vec{x},t)$ and consider $\vec{\nabla} \cdot \vec{j} \Rightarrow$

$$\vec{\nabla} \cdot \vec{j} = \frac{\hbar}{m} \vec{\nabla} \left[\mathrm{Im} \left(\Psi^* \vec{\nabla} \Psi \right) \right] = -\frac{i\hbar}{2m} \vec{\nabla} \left[\Psi^* \vec{\nabla} \Psi - (\vec{\nabla} \Psi^*) \Psi \right] = -\frac{i\hbar}{2m} \left[\cancel{\vec{\nabla} \Psi^* \cdot \vec{\nabla} \Psi} + \Psi^* \Delta \Psi - (\Delta \Psi^*) \Psi - \cancel{(\vec{\nabla} \Psi^*)(\vec{\nabla} \Psi)} \right] = \frac{\hbar}{m} \mathrm{Im} \left[(\Delta \Psi) \Psi^* \right]$$

$\Downarrow$

$$\boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0}$$

$\Rightarrow$ continuity equation $\Downarrow$ compare with charge conserv. in E&M, fluid dynamics etc.

$\Rightarrow$ conservation of the probability

What is the physical meaning of $\vec{j}$?

$\Downarrow$

We know that $\int_{V_0} d\vec{x} \, \rho(\vec{x},t)$ is a probability to find a particle in volume V_0,

$$\int_{\text{all space}} \rho(\vec{x},t) \, d\vec{x} = 1$$

What about $\int \vec{j}(\vec{x},t)\,d\vec{x} = -\frac{i\hbar}{2m}\int_{\substack{\text{all}\\ \text{space}}} [\psi^* \vec{\nabla}\psi -$

$- (\vec{\nabla}\psi^*)\psi]\,d\vec{x} =$

$$= \frac{1}{2m}\int_{\substack{\text{all}\\ \text{space}}} [\psi^* \underbrace{(-i\hbar\vec{\nabla}\psi)}_{\text{"}\vec{p}\psi} + \underbrace{(i\hbar\vec{\nabla}\psi^*)}_{\text{"}\vec{p}^*\psi^*}\psi]\,d\vec{x} =$$

$$= \frac{1}{2m}\int_{\substack{\text{all}\\ \text{space}}} \underbrace{\left(\psi^*(\vec{p}\psi) + (\vec{p}^*\psi^*)\psi\right)}_{a+ib+a-ib=2a} d\vec{x} =$$

$$= \frac{1}{2m}\cdot 2\,\mathrm{Re}\int_{\substack{\text{all}\\ \text{space}}} \psi^*(\vec{x},t)\,\vec{p}\,\psi(\vec{x},t)\,d\vec{x} =$$

$$= \frac{1}{m}\langle\vec{p}\rangle_t$$ ← expectation value of the momentum operator at time t

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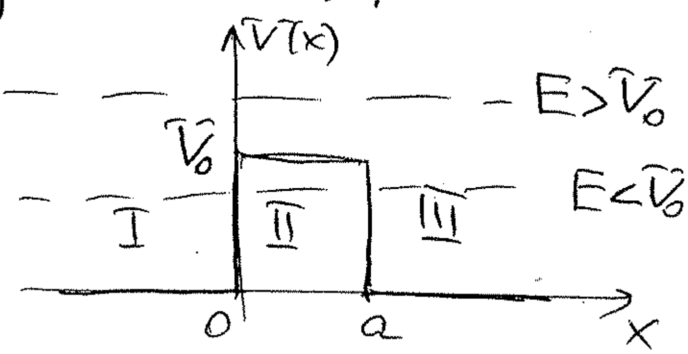
Tunneling

Consider a particle moving in $V(x)$:

$$V(x) = \begin{cases} 0, & x<0 \\ V_0, & 0<x<a \\ 0, & x>a \end{cases}$$

$(V_0 > 0)$



Classically: particle reflected if $E < V_0$
and transmitted if $E > V_0$

QM : ? $\Rightarrow$ 1D scattering problem

$$\Psi_{I}(x) = Ae^{ikx} + Be^{-ikx} \qquad (x<0)$$
$$\Psi_{III}(x) = Ce^{ikx} + De^{ikx} \qquad (x>a)$$
$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$\Psi_{II}(x) \rightarrow$ depends on whether $E > V_0$ or $E < V_0$

Let's specify that the particle is incident on the barrier from the left $\Rightarrow$ then there is nothing at large $x > 0$ to cause a reflection (i.e. e^{-ikx} term at $x>a$) $\Rightarrow D = 0$

Now look for transmission and reflection characteristics of the barrier :

reflection coefficient $R = \left|\frac{B}{A}\right|^2$

transmission coefficient $T = \left|\frac{C}{A}\right|^2$ $\Rightarrow$

Probability current densities: 5

$x<0$: $\quad j = -\frac{i\hbar}{2m}\left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right] =$

$$= \frac{\hbar}{m}\,\mathrm{Im}\Big[\underbrace{\psi^* \frac{d\psi}{dx}}_{\parallel}\Big] = \underline{\frac{\hbar}{m}k\left(|A|^2 - |B|^2\right)}$$

$$\left(A^* e^{-ikx} + B^* e^{ikx}\right)\cdot ik\left(A e^{ikx} - B e^{-ikx}\right) =$$

$$= ik\Big(|A|^2 - |B|^2 \underbrace{- A^* B e^{-2ikx} + B^* A e^{2ikx}}_{\parallel}\Big)$$

$$a + ib - a + ib = 2ib =$$

$$= 2i\,\mathrm{Im}\left[B^* A e^{2ikx}\right]$$

$x>a$: $\quad \underline{j = \frac{\hbar k}{m}|C|^2}$

$v = \frac{\hbar k}{m}$; $v|A|^2$; $v|B|^2$; $v|C|^2$

particle velocity; incident intensity; reflected intensity; transmitted intensity

reflection coefficient $R = \frac{|B|^2}{|A|^2}$

transmission coefficient $T = \frac{|C|^2}{|A|^2}$

independent of the normalization of ψ

1) $E < V_0$

$$\psi_{II}(x) = F e^{\varkappa x} + G e^{-\varkappa x}, \quad 0<x<a$$

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

Match boundary conditions:

$\psi(x)$, $\psi'(x)$ are continuous at $x=0$ and $x=a$ $\Rightarrow$

$$R = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2 \varkappa a}\right]^{-1}$$

$$T = \left[1 + \frac{V_0^2 \sinh^2 \varkappa a}{4E(V_0 - E)}\right]^{-1}$$

Show this for Homework!

$R + T = 1$ (conservation of the probability flux)

$T \neq 0 \Rightarrow$ barrier penetration, or tunneling

If $E \to 0 \Rightarrow T \to 0$

If $E \to V_0$ (but still $E < V_0$) $\Rightarrow \varkappa a = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\, a = \underset{\downarrow}{} 0$

$\Rightarrow \sinh^2 \varkappa a \approx (\varkappa a)^2 = \frac{2m}{\hbar^2}(V_0 - E)\, a^2$

Then $T = \left[1 + \frac{V_0 m a^2}{2\hbar^2}\right]^{-1}$

a measure of the "opacity" of the barrier (the larger V_0 and the wider $a \Rightarrow$ smaller T)

Classical limit!

$\hbar \to 0 \Rightarrow T = 0$!

2) $E > V_0$

$$\psi_{II}(x) = Fe^{ik'x} + Ge^{-ik'x}, \quad 0 < x < a$$

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

$$R = \left[1 + \frac{4E(E-V_0)}{V_0^2 \sin^2 k'a}\right]^{-1}$$

$$T = \left[1 + \frac{V_0^2 \sin^2 k'a}{4E(E-V_0)}\right]^{-1}$$

derive (Homework)!

Important: $T < 1$! $\Leftarrow$ in contradiction to the classical prediction!!

$T = 1$ only if $\underbrace{k'a = \pi + \pi n = \pi n'}_{}$ ← integer

condition of destructive interference between the reflections at $x = 0$ and $x = a$

At $E \gg V_0 \Rightarrow T \to 1$

Physical examples of tunneling:
- α-particle emission from a nucleus
- electron emission from metal
- scanning tunneling microscope

See Nature paper $\Rightarrow$