B. Continuity Equation in Quantum Mechanics

Seen in Electromagnetic Theory that

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0 \quad \text{(continuity equation)} \quad (3)$$

ρ = charge density ($\rho(\vec{r})\, d^3r$ = charge in d^3r volume element at $\vec{r}$)

$\vec{J}$ = current density

some volume [boundary needs not be physical]

Meaning:

[Change in charges in Volume per unit time] balanced by [current through the surface of the volume (in and out: Net)]

Back to QM: $\psi^*(\vec{r})\,\psi(\vec{r}) = \underbrace{|\psi(\vec{r})|^2}$ is analogous to ρ

[physical meaning in $|\psi(\vec{r})|^2 d^3r$] (c.f. $\rho(\vec{r})d^3r$)

$$\boxed{\begin{array}{l}\text{Question: Is there a continuity equation like (3) in Quantum Mechanics?} \\ \text{i.e. } \dfrac{\partial}{\partial t}(\psi^*\psi) + \vec{\nabla}\cdot\underbrace{[\text{something}]}_{\text{what is it?}} = 0 \quad [?]\end{array}}$$

Let's start with $\dfrac{\partial}{\partial t}(\psi^*\psi) = \psi^*\dfrac{\partial \psi}{\partial t} + \psi\dfrac{\partial \psi^*}{\partial t}$

TDSE: $i\hbar\dfrac{\partial \psi}{\partial t} = \hat{H}\psi \Rightarrow i\hbar\dfrac{\partial \psi}{\partial t} = -\dfrac{\hbar^2}{2m}\nabla^2\psi + V\psi$ [real V]

thus, $-i\hbar\dfrac{\partial \psi^*}{\partial t} = -\dfrac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*$

$$\frac{\partial}{\partial t}(\psi^*\psi) = \psi^*\left(\frac{-\hbar}{2mi}\nabla^2\psi\right) + \psi\left(\frac{\hbar}{2mi}\nabla^2\psi^*\right) \qquad \text{(Ex.)}$$

$$= \frac{-\hbar}{2mi}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

$$\boxed{\begin{aligned} \text{But } \psi^*\nabla^2\psi - \psi\nabla^2\psi^* &= \psi^*\nabla^2\psi + (\nabla\psi)\cdot(\nabla\psi^*) - (\nabla\psi)\cdot(\nabla\psi^*) - \psi\nabla^2\psi^* \\ &= \vec{\nabla}\cdot\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right] \end{aligned}}$$

$$\therefore \frac{\partial}{\partial t}(\psi^*\psi) = -\vec{\nabla}\cdot\left[\frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)\right] \qquad (4) \qquad \text{(done!)}$$

$$\therefore \boxed{\vec{J} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) \quad \text{(\underline{probability current density})}} \quad (5)$$

Eq. (4) is continuity equation in QM

Eq. (5) gives probability current density $\vec{J}$ in QM

Key Results:

$$\frac{\partial}{\partial t}(\psi^*\psi) + \vec{\nabla}\cdot\left[\frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)\right] = 0 \quad (4)$$

Continuity Equation

$$\vec{J} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*) \quad (5)$$

Probability current density

a vector

[$\nabla\psi$, $\nabla\psi^*$ are vectors] (gradient of a scalar is a vector)

- Work for any ψ (generally any $\Psi(\vec{x},t)$)
- 3D : $\nabla\psi$ (gradient of ψ) $= \hat{i}\frac{\partial}{\partial x}\psi + \hat{j}\frac{\partial}{\partial y}\psi + \hat{k}\frac{\partial}{\partial z}\psi$
- $\underbrace{\text{1D}}_{\text{taken as } x}$ version of $\vec{J}$: $\nabla \rightarrow \hat{i}\frac{\partial}{\partial x}$

still carries a direction

$$\boxed{\begin{array}{l}\text{1D Version of } \vec{J} \text{ (formally } \nabla \to \hat{i}\frac{\partial}{\partial x}) \\ \vec{J} = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial}{\partial x}\psi - \psi \frac{\partial}{\partial x}\psi^*\right)\hat{i}\end{array}}$$

(5a) [often used in tunneling problems]

<u>Example</u>: $\psi_k = A\, e^{ikx}$ (or $A\, e^{ikx - i\omega(k)t}$) [same result]

$$J_x = \frac{\hbar}{2mi}\left(|A|^2 e^{-ikx}(ik)e^{ikx} - |A|^2 e^{ikx}(-ik)e^{-ikx}\right)$$ [there is $\hat{i}$ for direction]

$$= \frac{\hbar}{2mi}\left(2ik|A|^2\right) = \underbrace{\frac{\hbar k}{m}|A|^2}_{\text{Result}} = \frac{p}{m}|A|^2 = \underbrace{v}_{\text{velocity}}|A|^2 \quad (6)$$

<u>Makes sense!</u>

$\psi_k \sim A\, e^{ikx}$ travels with momentum $p = \hbar k$

mass $m \Rightarrow$ travels with $v = \frac{\hbar k}{m}$

$\vec{J} = \frac{\hbar k}{m}|A|^2\,\hat{i}$

Prob. density $\sim |A|^2$

For electron with charge $(-e)$ in ψ_k, <u>Current Density $\vec{J}_e$</u> is:

$$J_{e,x} = (-e)\frac{\hbar}{2mi}\left(\psi^*\frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^*\right)$$

this is the "J" in EM theory

gives $\vec{J}_e = (-e)\frac{\hbar k}{m}|A|^2\,\hat{i}$ (useful in solid state/semiconductor physics)

- How about $\psi_{-k} = B e^{-ikx}$? Ex.

$$\vec{J} = -\frac{\hbar k}{m}|B|^2\,\hat{i}$$

"$-\hat{i}$" means moving in direction toward negative x

could have guessed it by physical sense

- How about $\psi(x) = A e^{ikx} + B e^{-ikx}$?

Plug into $\vec{J} = \frac{\hbar}{2mi} \underbrace{\left(\psi^* \nabla \psi - \psi \nabla \psi^* \right)}_{\text{gives many terms (Ex.)}}$. (5)

But the answer is simple! (Non-trivial, but make sense)

$$\vec{J} = \underbrace{|A|^2 \frac{\hbar k}{m} \hat{i}}_{\text{one direction}} - \underbrace{|B|^2 \frac{\hbar k}{m} \hat{i}}_{\text{opposite direction}} \quad (7)$$ [Try it out!]

[Need to use Eq.(7) in tunneling problem]

- How about stationary state such as $A \sin\left(\frac{\pi x}{L}\right)$ as in 1D Box?

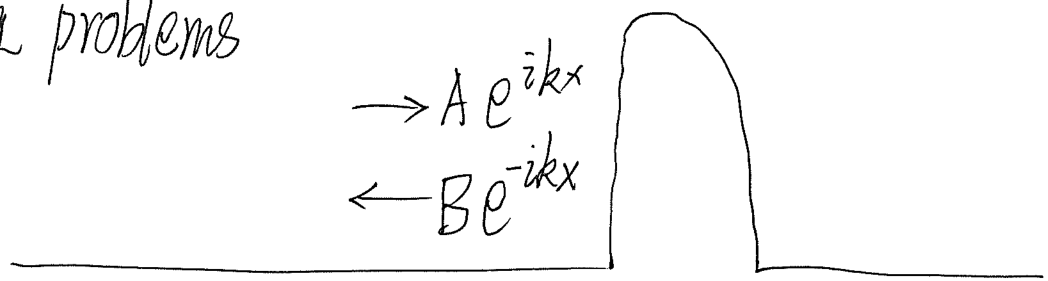
$J = 0$ (Ex.)

Take-Home message

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$

has corresponding $\vec{J} = |A|^2 \frac{\hbar k}{m} \hat{i} - |B|^2 \frac{\hbar k}{m} \hat{i}$

This is why in tunneling problems



is usually drawn

with $A e^{ikx}$ representing an incident wave [actually an incident probability current density in $+\hat{i}$ direction] and $B e^{-ikx}$ representing a reflected wave [a reflected probability current density in $-\hat{i}$ direction].

Remarks

- Concept of $\vec{J} = \frac{\hbar}{2mi}(\Psi^* \vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*)$ is important in applications (transport properties of materials) and in basic quantum mechanics

- Many non-trivial ideas

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

  - E.g. Particle in a box

    Stationary (energy eigenstate) state $\Psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-iE_n t/\hbar}$

    What is $\vec{J}$?

  - E.g. $\Psi(x,t) = A_1\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)e^{-iE_1 t/\hbar} + A_2\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)e^{-iE_2 t/\hbar}$

    What is $\vec{J}$? What are $|\Psi|^2$ and $\frac{\partial}{\partial t}|\Psi|^2$?

- Wavefunction with a <u>spatially dependent</u> <u>phase</u>

$$\psi(x) = e^{i\delta(x)} \underbrace{|\phi(x)|}_{\text{real by definition}} \quad ; \quad \delta(x) \text{ is spatially dependent}$$

OR $$\psi(\vec{x}) = e^{i\delta(\vec{x})} \overbrace{|\phi(\vec{x})|}^{\text{real by definition}} \quad ; \quad \delta(\vec{x}) \text{ is spatially dependent}$$

What is $\vec{J}$?

$$\left[\vec{J} = \frac{\hbar}{m} |\phi(\vec{x})|^2 \underbrace{\vec{\nabla}\delta(\vec{x})}_{\vec{\nabla}\delta(\vec{x}) \text{ leads to } \vec{J}\,!} \right]$$