6/10/2025

# Day 23. Time-dependent S.E. & the continuity equation

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle \quad — ①$$

given $\quad |\Psi(t=t_0)\rangle \equiv |\Psi_0\rangle \quad — ②$

Since both $|\Psi(t)\rangle$ and $|\Psi_0\rangle$ are in the same Hilbert space, we can think of an operator that connects the two:

$$\hat{U}(t,t_0) : |\Psi(t)\rangle = \hat{U}(t,t_0)|\Psi_0\rangle \quad — ③$$

Substituting this in ① yields.

$$i\hbar \frac{\partial}{\partial t}\hat{U}(t,t_0)|\Psi_0\rangle = \hat{H}(t)\hat{U}(t,t_0)|\Psi_0\rangle \quad — ④$$

Since $|\Psi_0\rangle$ could be any arbitrary starting state we have:

$$\boxed{i\hbar \frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0) \quad — ⑤}$$

Let's assume for the moment that $\hat{H}(t)$ is time-independent. In this case, (4) has a very straightforward solution:

$$\hat{U}(t, t_0) = \exp\left(-i \frac{\hat{H}}{\hbar}(t-t_0)\right) \quad \text{--- (5)}$$

as can be checked by substitution.

$\hat{U}$ is called a time-propagation operator.

Assuming that, if $|\Psi_0\rangle$ is normalized, so is $|\Psi(t)\rangle$ we get that

$$1 = \langle \Psi(t) | \Psi(t) \rangle$$

$$= \langle \Psi_0 | \hat{U}^\dagger(t, t_0) \hat{U}(t, t_0) | \Psi_0 \rangle$$

$$= \langle \Psi_0 | \Psi_0 \rangle \quad \text{--- (6)}$$

$$\Rightarrow \hat{U}^\dagger(t, t_0) \hat{U}(t, t_0) = \hat{1} \quad \text{--- (7)}$$

i.e. $\hat{U}$ is a unitary operator.

From the definition of $\hat{U}$, we must also have that,

$$|\Psi_0\rangle = \hat{U}(t_0, t)\,|\Psi(t)\rangle \quad -(8)$$

But also,

$$|\Psi_0\rangle = \hat{U}^{-1}(t, t_0)\,|\Psi(t)\rangle \quad -(9)$$

$$= \hat{U}^{\dagger}(t, t_0)\,|\Psi(t)\rangle \quad -(10)$$

$\therefore$ Comparing (8) and (9) we have that,

$$\hat{U}^{\dagger}(t, t_0) = \hat{U}(t_0, t) \quad -(11)$$

reverse propagation in time.

E.g. A particle in a 1-d box starts out at $t=0$ in a superposition of $n=1, n=2$

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{\sqrt{2}}|\psi_2\rangle \quad -(12)$$

What is the state after time $t$?

$$|\Psi(t)\rangle = \hat{U}(t,0)\,|\Psi_0\rangle$$

$$= \exp\left(-i\frac{\hat{H}t}{\hbar}\right)\left\{\frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{\sqrt{2}}|\psi_2\rangle\right\}$$

energy eigenfns

$$= \frac{1}{\sqrt{2}}\left\{\exp\left(-i\frac{E_1 t}{\hbar}\right)|\psi_1\rangle + \exp\left(-i\frac{E_2 t}{\hbar}\right)|\psi_2\rangle\right\}$$

$$\left(\because f(\hat{H})|\psi_1\rangle = f(E_1)|\psi_1\rangle\right) \qquad \text{— (13)}$$

Similarly, a free particle in 1-d starting from an eigenstate $|\psi_p\rangle$ evolves as:

$$|\Psi(t)\rangle = \exp\left(-i\frac{\hat{H}t}{\hbar}\right)|\psi_p\rangle$$

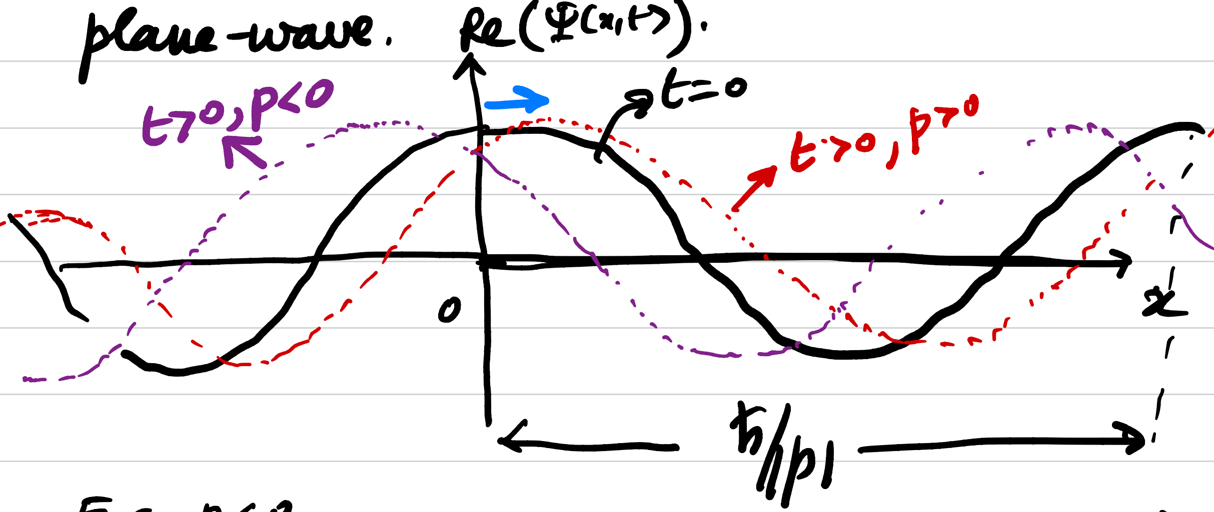
$$= \exp\left(-i\frac{p^2}{2m\hbar}t\right)|\psi_p\rangle \qquad \text{— (14)}$$

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-i\frac{p^2}{2m\hbar}t\right)\exp\left(i\frac{p}{\hbar}x\right)$$

$$\equiv \frac{1}{\sqrt{2\pi\hbar}} \exp\left(i\left(\frac{p}{\hbar}x - \omega_p t\right)\right) \quad \text{— (15)}$$

$$\left(\text{where } \omega_p = \frac{p^2}{2m\hbar}\right)$$

For $p>0$, this is a right-moving plane-wave.




For $p<0$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-i\left(\frac{|p|}{\hbar}x + \omega t\right)\right)$$

$\Rightarrow$ left moving wave.

This aligns with our general notion of particle motion and sign of momentum.

We will see what happens for time-dependent potentials later in this course.

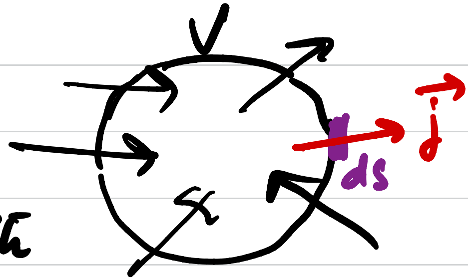
Continuity eqn..

In classical electrodynamics, we have the continuity equation describing the local conservation of charge.

$$\frac{\partial \rho(\vec{r},t)}{\partial t} = -\vec{\nabla}\cdot\vec{j}(\vec{r},t) \quad \text{(1b)}$$

where $\rho(\vec{r},t)$ is the instantaneous charge density

$\vec{j}(\vec{r},t)$ is the current density = amount of charge flowing per unit time across a unit area with normal $\parallel \vec{j}$.




Total charge inside the volume can change due to both in-flow and out-flow.

$$Q(t) = \int_V \rho(\vec{r},t)\, d^3r \qquad \text{— (17)}$$

Net outwards flux across the boundary of V.

$$= \oint_S \underbrace{\vec{j}(\vec{r},t)\cdot d\vec{s}} \qquad \text{— (18)}$$

amount flowing across $d\vec{s}$ per unit time.

If no other processes change Q(t) then we have:

$$\frac{dQ(t)}{dt} + \oint_S \vec{j}(\vec{r},t)\cdot d\vec{s} = 0 \qquad \text{— (19)}$$

More locally, we can use the Gauss divergence theorem in (18)

$$\text{Net flux} = \oint_S \vec{j} \cdot d\vec{s} = \int_V \vec{\nabla} \cdot \vec{j} \, d^3r \qquad (20)$$

and $$\frac{dq}{dt} = \int_V d^3r \, \frac{\partial \rho(\vec{r}, t)}{\partial t} \qquad (21)$$

$$\therefore \int_V d^3r \left[ \frac{\partial \rho(\vec{r}, t)}{\partial t} + \vec{\nabla} \cdot \vec{j}(\vec{r}, t) \right] = 0 \qquad (22)$$

$$\Rightarrow \boxed{\frac{\partial \rho(\vec{r}, t)}{\partial t} = - \vec{\nabla} \cdot \vec{j}(\vec{r}, t)} \qquad (23)$$

This is the local version of the continuity equation indicated in (19).

→ Disappearance of charge from any (infinitesimal) region is due to an out-flow of charge into other (neighbouring) regions

→ Total charge is conserved (over time).

7/10/2025 Day 24 Continuity Equation

In the context of QM, a similar conservation property holds for the probability, for instance, of finding a particle in a volume $d^3r$ around $\vec{r}$ at any time. This is ensured by normalization of the state.

$$\langle \Psi(t) | \Psi(t) \rangle = 1 \qquad — (24)$$

$$\Rightarrow 1 = \int d^3r \, \langle \Psi(t) | \vec{r} \rangle \langle \vec{r} | \Psi(t) \rangle$$

$$= \int d^3r \, \Psi^*(\vec{r},t) \, \Psi(\vec{r},t)$$

$$\equiv \int d^3r \, P(\vec{r},t) \qquad — (25)$$

probability density. (like charge density)

So can we derive an analogous continuity equation in QM?

Yes.

Consider the TDSE in position representation. (for 1-particle in 3-d)

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r},t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r},t) + V(\vec{r},t)\Psi(\vec{r},t) \quad -(26)$$

Taking complex conjugate on both sides we get.

$$-i\hbar \frac{\partial}{\partial t} \Psi^*(\vec{r},t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi^*(\vec{r},t) + V(\vec{r},t)\Psi^*(\vec{r},t) \quad -(27)$$

Here, V is assumed to be real as is required for Hermiticity of $\hat{H}$.

$\Psi^* \times (26) - \Psi \times (27) \Rightarrow$

$$i\hbar \left[ \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \right] = -\frac{\hbar^2}{2m} \left[ \Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^* \right] \quad -(28)$$

$$\Rightarrow \quad i\hbar \frac{\partial P(\vec{r},t)}{\partial t}$$

$$= \frac{-\hbar^2}{2m}\Big[ \Psi^* \nabla^2 \Psi + (\vec{\nabla}\Psi^*)\cdot(\vec{\nabla}\Psi) - (\vec{\nabla}\Psi)\cdot(\vec{\nabla}\Psi)^* - \Psi \nabla^2 \Psi^* \Big]$$

$$= \frac{-\hbar^2}{2m}\Big[ \vec{\nabla}\cdot\big( \Psi^* \vec{\nabla}\Psi - \Psi \vec{\nabla}\Psi^* \big) \Big] \quad \text{--- (29)}$$

where we have used the identity.

$$\left.\begin{aligned} \vec{\nabla}\cdot\big(f(\vec{r})\vec{A}(\vec{r})\big) &= \vec{\nabla}f(\vec{r})\cdot\vec{A}(\vec{r}) + f(\vec{r})\,\vec{\nabla}\cdot\vec{A}(\vec{r}) \\ \& \quad \vec{\nabla}\cdot\vec{\nabla}f &= \nabla^2 f \end{aligned}\right\} \quad (30)$$

(29) $\Rightarrow$ $$\boxed{\frac{\partial P(\vec{r},t)}{\partial t} = -\vec{\nabla}\cdot\vec{j}(\vec{r},t)} \quad \text{--- (31)}$$

where $$\boxed{\vec{j}(\vec{r},t) \equiv \frac{\hbar}{2mi}\left[\Psi^*(\vec{r},t)\,\vec{\nabla}\,\Psi(\vec{r},t) - \Psi(\vec{r},t)\,\vec{\nabla}\,\Psi^*(\vec{r},t)\right]} \quad \text{--- (32)}$$

is the probability current density.

Since $\quad z - z^* = 2i\,\mathrm{Im}(z)$ — (33)

we can also write (32) as

$$\boxed{\vec{j}(\vec{r},t) = \mathrm{Im}\left\{\frac{\hbar}{m}\,\Psi^*(\vec{r},t)\,\vec{\nabla}\,\Psi(\vec{r},t)\right\}} \quad \text{--- (34)}$$

Since total probability is always conserved,

$$\lim_{V\to\infty} \frac{d}{dt} \int_V d^3r \, P(\vec{r},t) = -\int_V d^3r \, \vec{\nabla}\cdot\vec{j}(\vec{r},t)$$

$$= -\int_{S(V)} \vec{j}(\vec{r},t)\cdot d\vec{S}$$

$$= 0 \qquad \text{— (35)}$$

$\Rightarrow$ The net probability out-flux at the boundaries (infinities) vanishes and, even, locally, $\lim_{|\vec{r}|\to\infty} \vec{j}(\vec{r},t) \to 0$ — (36)

Examples.

(1) $$\psi_{\vec{p}}(\vec{r},t) = \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3 \exp\left( i\left(\frac{\vec{p}\cdot\vec{r}}{\hbar} - \omega_{\vec{p}} t\right)\right)$$

where $\omega_p = \dfrac{p^2}{2\hbar m}$ — (37)

$$\vec{\nabla}\psi_{\vec{p}}(\vec{r},t) = \left(\frac{i\vec{p}}{\hbar}\right)\psi_{\vec{p}}(\vec{r},t) \quad \text{— (38)}$$

$$\Rightarrow \quad \psi^*_{\vec{p}}(\vec{r},t)\,\vec{\nabla}\psi_{\vec{p}}(\vec{r},t) = \frac{i\vec{p}}{\hbar}\left(\frac{1}{2\pi\hbar}\right)^3$$

$$\Rightarrow \vec{j}(\vec{r},t) = \mathrm{Im}\left\{\frac{\hbar}{m}\psi^*_{\vec{p}}(\vec{r},t)\,\vec{\nabla}\psi_{\vec{p}}(\vec{r},t)\right\}$$

$$= \frac{\vec{p}}{m}\cdot\frac{1}{(2\pi\hbar)^3} \quad \text{— (39)}$$

$\Rightarrow \vec{\nabla}\cdot\vec{j} = 0 \quad \Longleftrightarrow \quad \rho(\vec{r},t) = 1/(2\pi\hbar)^3$

$$\Rightarrow \frac{\partial\rho(\vec{r},t)}{\partial t} = 0$$

Note that (39) also means.

$$\vec{j}(\vec{r},t) = P(\vec{r},t)\left(\frac{\vec{p}}{m}\right) = P(\vec{r},t)\,\vec{v} \quad \text{— (40)}$$

which agrees with the classical notion of current density.

(2) $$\psi(\vec{r},t) = \phi(\vec{r})\, e^{-iE/\hbar\, t} \quad \text{— (41)}$$

$$\vec{\nabla}\psi(\vec{r},t) = \left(\vec{\nabla}\phi(\vec{r})\right) e^{-iE/\hbar\, t} \quad \text{— (42)}$$

$$\Rightarrow \psi^* \vec{\nabla}\psi = \phi^*(\vec{r})\,\vec{\nabla}\phi(\vec{r}) \quad \text{— (43)}$$

If $\phi(\vec{r}) \in \mathbb{R}$, then $\psi^*\vec{\nabla}\psi \in \mathbb{R}$.

$$\Rightarrow \boxed{\vec{j}(\vec{r},t) = 0} \quad \text{— (44)}$$

Thus, the current density associated with real wavefunctions or wavefunction with only separable complex time parts is zero.

③ $\psi(x,t) = A(t)\, e^{ipx/\hbar} + B(t)\, e^{-ipx/\hbar}$

$$\psi^* \nabla \psi = \left(A^* e^{-ipx/\hbar} + B^* e^{ipx/\hbar}\right)$$

$$\frac{ip}{\hbar}\left(A\, e^{ipx/\hbar} - B\, e^{-ipx/\hbar}\right)$$

$$= i\left(|A|^2 - |B|^2\right)\frac{p}{\hbar}$$

$$+ ip/\hbar \left[AB^* e^{i2px/\hbar} - A^* B e^{-i2px/\hbar}\right]$$

$$= i\left(|A|^2 - |B|^2\right)p/\hbar$$

$$- 2p/\hbar \,\mathrm{Im}\left\{AB^* e^{i2px/\hbar}\right\} \quad \text{— (45)}$$

$$\Rightarrow \frac{\hbar}{m}\mathrm{Im}\left\{\psi^* \nabla \psi\right\} = \left(|A|^2 - |B|^2\right)\frac{p}{m}$$

$$= j(x,t), \quad \text{— (46)}$$