A, A is hermitian

$$Af = A^{\dagger}f, \quad f \in D(A)$$

$$A = A^{\dagger} \text{ in } D(A)$$

1. If A is hermitian, A^n is hermitian too $(n = 0, \pm 1, \pm 2, \ldots)$

Proof:

$$\underline{(A^n)^{\dagger}} = (A^{\dagger})^n \overset{A=A^{\dagger}}{=\!=} \underline{A^n}$$

2. Let us assume that A and B are hermitian.

AB is hermitian if
$[A,B]=0$.

Proof:

$$(AB)^{\dagger} = B^{\dagger}A^{\dagger} = BA$$

$$[A,B]=0, \quad AB-BA=0$$

$$AB=BA$$

$$(AB)^{\dagger} = BA = AB$$

3. If A and B are hermitian, $\alpha A+\beta B$ is hermitian too as long as α and β are real numbers.

Proof:

$$(\alpha A+\beta B)^\dagger = \alpha^* A^\dagger + \beta^* B^\dagger$$

$$= \alpha A + \beta B$$

We used: $A = A^\dagger$, $B = B^\dagger$, $\alpha = \alpha^*$, $\beta = \beta^*$

OPERATORS IN QUANTUM MECHANICS

$$F(q_1, \ldots, q_f, p_1, \ldots, p_f, t)$$

$$\hat{F} = F(\hat{q}_1, \ldots, \hat{q}_f, \hat{p}_1, \ldots, \hat{p}_f, t)$$

Let us start with $\hat{q}_\ell$ and $\hat{p}_\ell$.

$$\boxed{\hat{q}_\ell \text{ and } \hat{p}_\ell \text{ are hermitian}}$$

$$\underline{(f, Ag) = (Af, g)}$$

$$\mathcal{H} = L^2(\Gamma)$$

$$(\varphi, \psi) = \int_\Gamma \varphi^* \psi \, d\tau$$

$$\underline{(\varphi, \hat{q}_\ell \psi)} = \int_\Gamma \varphi^* (\hat{q}_\ell \psi) \, d\tau$$

$$= \int_\Gamma \varphi^* q_\ell \psi \, d\tau$$

$$= \int_\Gamma (q_\ell \varphi)^* \psi \, d\tau$$

$$= \int_{\Gamma} (\hat{q}_\ell \varphi)^* \chi \, d\tau$$

$$= (\hat{q}_\ell \varphi, \chi)$$

$$\hat{p}_\ell = \frac{\hbar}{i} \frac{\partial}{\partial q_\ell} = -i\hbar \frac{\partial}{\partial q_\ell}$$

We must distinguish between, e.g., $\hat{p}_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$, $x \in (-\infty, \infty)$, and, say, $\hat{p}_\varphi = \frac{\hbar}{i} \frac{\partial}{\partial \varphi}$, $\varphi \in [0, 2\pi)$

(there are other cases, e.g.,

$$\hat{p}_r = \frac{\hbar}{i}\frac{\partial}{\partial r}, \quad r \in [0,\infty))$$

$$\boxed{\begin{gathered}\lim_{|x|\to\infty} \psi(x,\ldots) = 0 \\ \psi(\varphi=0) = \psi(\varphi=2\pi)\end{gathered}}$$

$\hat{p}_x$:

$$\underline{(\varphi, \hat{p}_x\psi)} = \int_{\mathbb{R}^3} \varphi^*(\hat{p}_x\psi)\,d\tau$$

$d\tau$: dxdydz

$$= \frac{\hbar}{i}\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dx\, \varphi^* \frac{\partial\psi}{\partial x}$$

$$= \frac{\hbar}{i}\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \cancel{\left[\varphi^*\psi\Big|_{x=-\infty}^{x=+\infty}\right]} \to 0$$

$$- \int_{-\infty}^{\infty} dx \left(\frac{\partial \varphi}{\partial x}\right)^{*} \psi \Big]$$

dxdydz

$$= -\frac{\hbar}{i} \int_{\mathbb{R}^3} \left(\frac{\partial \varphi}{\partial x}\right)^{*} \psi \, d\tau$$

$$= \int_{\mathbb{R}^3} \left(\frac{\hbar}{i} \frac{\partial \varphi}{\partial x}\right)^{*} \psi \, d\tau$$

$$= \int_{\mathbb{R}^3} (\hat{p}_x \varphi)^{*} \psi \, d\tau$$

$$= (\hat{p}_x \varphi, \psi)$$

$$\hat{p}_\varphi = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}, \quad \varphi = [0, 2\pi)$$

$$f(\varphi), \; g(\varphi)$$

$$(f, \hat{p}_\varphi g) = \int_0^{2\pi} f^*(\hat{p}_\varphi g)\, d\varphi$$

$$= \frac{\hbar}{i}\int_0^{2\pi} f^* \frac{\partial g}{\partial\varphi}\, d\varphi$$

$$= \frac{\hbar}{i}\left[f^* g \Big|_{\varphi=0}^{\varphi=2\pi} - \int_0^{2\pi}\left(\frac{\partial f}{\partial\varphi}\right)^* g\, d\varphi \right]$$

0

$$f^*(\varphi=0)\,g(\varphi=0) = f^*(\varphi=2\pi)\,g(\varphi=2\pi)$$

$$= -\frac{\hbar}{i}\int_0^{2\pi}\left(\frac{\partial f}{\partial\varphi}\right)^* g\,d\varphi$$

$$= \int_0^{2\pi}\left(\frac{\hbar}{i}\frac{\partial f}{\partial\varphi}\right)^* g\,d\varphi$$

$$= \int_0^{2\pi}(\hat{p}_\varphi f)^* g\,d\varphi$$

$$= (\hat{p}_\varphi f, g)$$

$$[\hat{q}_k, \hat{p}_l] = i\hbar\,\delta_{kl}\,\mathbb{1}$$

unit operator

$$= i\hbar\,\delta_{kl}$$

$$[\hat{q}_k, \hat{p}_l]\cancel{\psi} = \hat{q}_k\hat{p}_l\psi - \hat{p}_l\hat{q}_k\psi$$

$$= \frac{\hbar}{i}\left(q_k\frac{\partial\psi}{\partial q_l} - \frac{\partial}{\partial q_l}q_k\psi\right)$$

$$= \frac{\hbar}{i}\left(\cancel{q_k\frac{\partial\psi}{\partial q_l}} - \underbrace{\frac{\partial q_k}{\partial q_l}}_{=\delta_{kl}}\psi - \cancel{q_k\frac{\partial\psi}{\partial q_l}}\right)$$

$$= -\frac{\hbar}{i}\,\delta_{kl}\psi = i\hbar\,\delta_{kl}\cancel{\psi}$$

$$[\hat{q}_k, \hat{p}_l] = i\hbar\,\delta_{kl}$$

$$[\hat{q}_k, \hat{q}_l] = 0$$

$$[\hat{p}_k, \hat{p}_l] = 0$$

In classical mechanics

$$\{q_k, p_l\} = \delta_{kl}$$

$$\{q_k, q_l\} = 0$$

$$\{p_k, p_l\} = 0$$

$$CM \longrightarrow QM$$

$$\{\ ,\ \} \longrightarrow \frac{1}{i\hbar}[\ ,\ ]$$

More complicated operators

- $\hat{V} = V(\hat{q}_1, \dots, \hat{q}_f, t)$

$$\hat{V}\psi = V\psi \qquad (V = V^*)$$

$$(\varphi, \hat{V}\psi) = \int_\Gamma \varphi^* (\hat{V}\psi)\, d\tau$$

$$= \int_\Gamma \varphi^* V \psi \, d\tau$$

$$\left(e^{i\omega t} \to e^{-\alpha t} \right)$$

$$\overset{V=V^*}{=} \int_\Gamma (V\varphi)^* \psi \, d\tau$$

$$= \int (\hat{V}\varphi)^* \chi \, d\tau$$

$$= (\hat{V}\varphi, \chi)$$

- $$\hat{T} = \sum_{j=1}^{3N} \frac{\hat{p}_j^2}{2m_j}$$ ✓

$$\hat{p}_j = \frac{\hbar}{i}\frac{\partial}{\partial x_j}$$

$$\hat{T} = -\sum_{j=1}^{3N} \frac{\hbar^2}{2m_j}\frac{\partial^2}{\partial x_j^2}$$ ✓

$\hat{p}_j$ is hermitian,

$\hat{p}_j^2$ is hermitian,

$\frac{\hat{p}_j^2}{2m_j}$ is hermitian,

sum of $\frac{\hat{p}_j^2}{2m_j}$ is hermitian

$\Downarrow$

$\hat{T}$ is hermitian.

$N=1$: $\hat{T} = -\frac{\hbar^2}{2m}\nabla^2$

$$\nabla^2 = -\frac{2m}{\hbar^2}\hat{T} = -\frac{1}{\hbar^2}\hat{\vec{p}}^{\,2}$$

hermitian

∇^2 is hermitian

- $\hat{H} = \hat{T} + \hat{V}$

hermitian hermitian

$\hat{H}$ is hermitian

- $\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$
$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$
$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

$$\hat{L}_x^\dagger = (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)^\dagger$$
$$= (\hat{y}\hat{p}_z)^\dagger - (\hat{z}\hat{p}_y)^\dagger$$
$$= \hat{p}_z^\dagger \hat{y}^\dagger - \hat{p}_y^\dagger \hat{z}^\dagger$$
$$= \hat{p}_z \hat{y} - \hat{p}_y \hat{z}$$
$$[\hat{z}, \hat{p}_y] = 0, \ [\hat{y}, \hat{p}_z] = 0$$

$$= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = \hat{L}_x$$

$$\hat{L}_x^\dagger = \hat{L}_x$$

$$\hat{L}_y^\dagger = \hat{L}_y$$

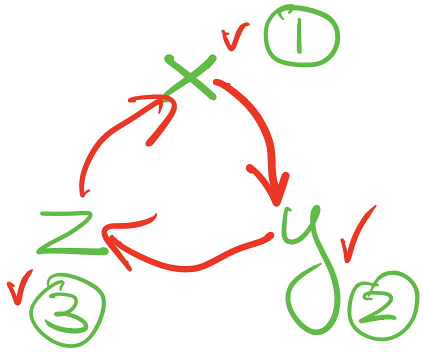
$$\hat{L}_z^\dagger = \hat{L}_z$$

$\hat{\vec{L}}$ is hermitian

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$



In CM: $\{L_x, L_y\} = L_z$ etc.

$$\{\ ,\ \} \longrightarrow \frac{1}{i\hbar}[\ ,\ ]$$

CM QM

$$L_1 = L_x,\quad L_2 = L_y,\quad L_3 = L_z$$

✓ $$[\hat{L}_i, \hat{L}_j] = i\hbar\, \varepsilon_{ijk} \hat{L}_k$$

ε_{ijk}: $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$

$$\varepsilon_{132} = \varepsilon_{321} = \varepsilon_{213} = -1$$

$$\checkmark \quad \vec{\hat{L}} \times \vec{\hat{L}} = i\hbar \vec{\hat{L}}$$

$$(\vec{\hat{L}} \times \vec{\hat{L}})_z =$$

$$= \hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x$$

$$= [\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

Sometimes we must be extra careful, since operators in QM do not commute.

Example:
Hamiltonian of a particle in electromagnetic field

In CM:

vector potential

$$H = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\varphi$$

scalar potential

We can write the following expressions:

$$H \stackrel{CM}{=} \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)\cdot\left(\vec{p} - \frac{q}{c}\vec{A}\right) + q\varphi$$

$$= \frac{\vec{p}^{\,2}}{2m} - \frac{q}{2mc}\underbrace{\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right)}_{\text{YES}} + \frac{q^2}{2mc^2}\vec{A}^{\,2} + q\varphi$$

$$= \frac{\vec{p}^{\,2}}{2m} - \frac{q}{mc}\left(\vec{p}\cdot\vec{A}\right) + \frac{q^2}{2mc^2}\vec{A}^{\,2} + q\varphi$$

NO

$$= \frac{\vec{p}^{\,2}}{2m} - \frac{q}{mc}\left(\vec{A}\cdot\vec{p}\right) + \frac{q^2}{2mc^2}\vec{A}^{\,2} + q\varphi$$

NO

We MUST make sure that $\hat{H}$ is HERMITIAN.

Is $\hat{\vec{p}} \cdot \hat{\vec{A}}$ hermitian ?

$$(\hat{\vec{p}} \cdot \hat{\vec{A}})^{\dagger} = (\hat{p}_x \hat{A}_x + \hat{p}_y \hat{A}_y + \hat{p}_z \hat{A}_z)^{\dagger}$$

$$= (\hat{p}_x \hat{A}_x)^{\dagger} + (\hat{p}_y \hat{A}_y)^{\dagger} + (\hat{p}_z \hat{A}_z)^{\dagger}$$

$$= \hat{A}_x^{\dagger} \hat{p}_x^{\dagger} + \hat{A}_y^{\dagger} \hat{p}_y^{\dagger} + \hat{A}_z^{\dagger} \hat{p}_z^{\dagger}$$

$$= \hat{A}_x \hat{p}_x + \hat{A}_y \hat{p}_y + \hat{A}_z \hat{p}_z$$

$$= \hat{\vec{A}} \cdot \hat{\vec{p}}$$

$$(\hat{\vec{p}} \cdot \hat{\vec{A}})^{\dagger} = \vec{A} \cdot \vec{p} \quad \checkmark$$

$\vec{p} \cdot \vec{A}$ is not hermitian

$$\hat{\vec{A}} = A(\hat{x}, \hat{y}, \hat{z}, t)$$

$$(\hat{\vec{A}} \cdot \hat{\vec{p}})^{\dagger} = \vec{p} \cdot \vec{A} \quad \checkmark$$

$$(\hat{\vec{p}} \cdot \hat{\vec{A}} + \hat{\vec{A}} \cdot \hat{\vec{p}})^{\dagger}$$

$$= (\hat{\vec{p}} \cdot \hat{\vec{A}})^{\dagger} + (\hat{\vec{A}} \cdot \hat{\vec{p}})^{\dagger}$$

$$= \hat{\vec{A}} \cdot \hat{\vec{p}} + \hat{\vec{p}} \cdot \vec{A}$$

$\hat{\vec{p}} \cdot \hat{\vec{A}} + \hat{\vec{A}} \cdot \hat{\vec{p}}$ is hermitian

$$\hat{H} = \frac{\hat{\vec{p}}^{2}}{2m} \checkmark - \frac{q}{2mc}(\hat{\vec{p}} \cdot \hat{\vec{A}} + \hat{\vec{A}} \cdot \hat{\vec{p}}) + \frac{q^2}{2mc^2}\vec{A}^2 \checkmark + q\varphi \checkmark$$

$$\hat{H}^{\dagger} = H$$

$\frac{1}{2}(B + B^{\dagger})$ is always hermitian

$$\frac{\hat{\vec{p}}^{\,2}}{2m} = -\frac{\hbar^2}{2m}\nabla^2 \quad \checkmark$$

$$\vec{p} = -i\hbar\vec{\nabla}$$

$$\cancel{\hat{\vec{p}}\cdot\hat{\vec{A}} = -i\hbar\vec{\nabla}\cdot\vec{A}} \quad !$$

$$(\hat{\vec{p}}\cdot\hat{\vec{A}})f =$$

$$= \Big[(\hat{p}_x\hat{A}_x)f + (\hat{p}_y\hat{A}_y)f$$

$$+ (\hat{p}_z \hat{A}_z) f \Big]$$

$$= -i\hbar \left[\frac{\partial}{\partial x}(A_x f) + \frac{\partial}{\partial y}(A_y f) + \frac{\partial}{\partial z}(A_z f) \right]$$

$$= -i\hbar \left[\underline{\frac{\partial A_x}{\partial x}} f + \underline{A_x \frac{\partial f}{\partial x}} + \underline{\frac{\partial A_y}{\partial y}} f + \underline{A_y \frac{\partial f}{\partial y}} + \underline{\frac{\partial A_z}{\partial z}} f + \underline{A_z \frac{\partial f}{\partial z}} \right]$$

$$= -i\hbar\left[\left(\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}\right)f\right.$$

$$\left. + (\vec{A} \cdot \vec{\nabla})f\right]$$

$$(\hat{\vec{p}} \cdot \hat{\vec{A}})f = -i\hbar\left(\vec{\nabla} \cdot \vec{A}\right.$$

$$\left. + \vec{A} \cdot \vec{\nabla}\right)f$$

$$\hat{\vec{p}} \cdot \hat{\vec{A}} = -i\hbar\left(\vec{\nabla} \cdot \vec{A}\, 1 + \vec{A} \cdot \vec{\nabla}\right)$$

$$\hat{\vec{A}} \cdot \hat{\vec{p}} = -i\hbar\, \vec{A} \cdot \vec{\nabla}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{iq\hbar}{2mc} \times$$

$$\times \left(\vec{\nabla}\cdot\vec{A}\,\mathbb{1} + 2\vec{A}\cdot\vec{\nabla} \right)$$

$$+ \frac{q^2}{2mc^2}\vec{A}^2 + q\varphi$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{iq\hbar}{mc}\vec{A}\cdot\vec{\nabla}$$

$$+ \frac{iq\hbar}{2mc}\left(\vec{\nabla}\cdot\vec{A}\right)\mathbb{1}$$

$$+ \frac{q^2}{2mc^2}\vec{A}^2 + q\varphi$$

DIRAC NOTATION

$(f,g) \rightarrow$ scalar product

$$(\varphi,\psi) = \int \varphi^* \psi \, d\tau$$

$$\underbrace{\langle \varphi | \psi \rangle}_{\text{bracket}} = (\varphi,\psi)$$

$\langle \varphi |$ = "bra"

$| \psi \rangle$ = "ket"

$$\underset{\text{bra}}{\langle \varphi |} \cdot \underset{\text{ket}}{| \psi \rangle} = \underset{\text{bracket}}{\langle \varphi | \psi \rangle}$$