Week 6 – Observables, Uncertainty

→ Complete sets of commuting observables

- Main motivation: We have $\hat{A} = \hat{A}^{\dagger} = \sum_{a \in \sigma_A} a \hat{P}_a$ and $\hat{B} = \hat{B}^{\dagger} = \sum_{b \in \sigma_B} b \hat{\Lambda}_b$ and $[\hat{A}, \hat{B}] = 0$, $[\hat{P}_a, \hat{\Lambda}_b] = 0$

  If both $\hat{A}$ and $\hat{B}$ are degenerate in the same spaces, you cannot completely describe the states in those eigenspaces via values measured for $\hat{A}$ and $\hat{B}$ alone.
- We need more observables (not degenerate in that space) to specify!

→ Examples

- Total energy of hydrogen atom (electrons): $\hat{H} |m, l, n, \sigma\rangle = E_n |n, l, m, \sigma\rangle$

  Here, we need to specify:
  - n, the principal quantum number / energy level
  - l, the orbital angular momentum
    (ranges from 0 to $n-1$, corresponds to shapes s, p, d, f, ...)
  - m, the magnetic quantum number
    (ranges from $-l$ to l, corresponds to orientation of orbitals
  - σ, the spin quantum number
    (intrinsic angular momentum, not momentum from motion in space)
    $\pm 1/2$

  Even if we fix n and l, we have an eigenspace with dimension $\dim(H_{n,l}) = 2(2l+1)$, since there are 2 possible spins and $2l+1$ possible m's.

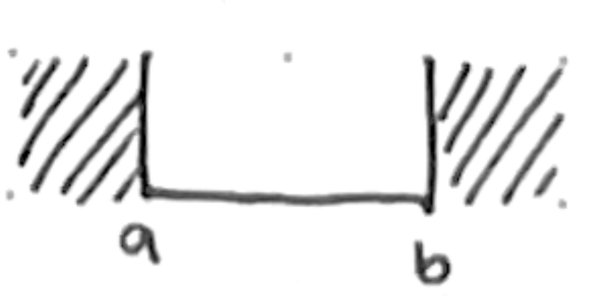
  If we also fix m, degeneracy $= 2$, etc.
- Total angular momentum^2

  $\hat{L}^2 | n, l, m, \sigma\rangle = \hbar^2 l(l+1) |n, l, m, \sigma\rangle$

→ This extra observable, $\hat{C}$, must commute with $\hat{A}$ and $\hat{B}$ also.

A set $\{\hat{A}, \hat{B}, \hat{C}, \dots\}$ whose eigenvalues identify a unique vector in the space is a CSCO.

→ Examples of CSCOs

- $\{\hat{H}\}$ for a particle in a box  $\hat{H} = \hat{P}^2/2m$ where $\hat{H}$ is defined for a suitably dense subset of $L^2([a,b])$ where it vanishes @ a and b.

  If we know $\hat{H}$'s eigenvalue $E_n = \hbar(n\pi)^2/(b-a)^2 2m$ we know the entire state.

etc...

- $\{\hat S_z\}$ in $\mathbb{C}^2$, knowing $\pm\frac{\hbar}{2}$ tells us $|\pm\rangle$ for sure.
- Any non-degenerate observable!
- $\{\hat L^2, \hat L_z\}$

Say our $\mathcal{H} = \text{span}\left\{ \frac{x^n y^m z^k}{\pi^{n+m+k}},\ n,m,k \in \mathbb{N} \right\}$ and

$$\langle f|g\rangle = \int_{-1}^{1}\int_{0}^{2\pi} d\cos\theta\, d\phi \cdot f^*(\theta,\phi)\, g(\theta,\phi)$$ (spherical harmonics...)

$\hat L^2$ gives you $\ell = 0,1,2,\ldots$ all $\ell > 0$ have many corresponding states.
$\hat L_z$ " " $m = -\ell, \ldots, \ell$ to specify

$\hat L^2 |f\rangle = \hbar^2 \ell(\ell+1)|f\rangle$, $\hat L_z |f\rangle = \hbar m |f\rangle$, so $|f\rangle$ is uniquely described up to a phase factor / normalization factor.

→ Closure relation

Note that just because $\mathbb{I} = \sum_i |i\rangle\langle i|$ for ONB $\{|i\rangle\}$, you <u>can't</u> say $\mathbb{I} = \sum_a \sum_b \sum_c |a,b,c\rangle\langle a,b,c|$ for some set of eigenvectors $|a,b,c\rangle$.

As in $|n,\ell,m,\sigma\rangle$, the eigenvalues need to be properly constrained. Not <u>all</u> combos of eigenvalues correspond to a state!

→ Non-Compatible Observables.

- Say $\hat A$ and $\hat B$ are observables that <u>may</u> not commute.

CASE 1:

$\langle\psi|\psi\rangle = 1$

$$|\psi\rangle \longrightarrow \boxed{\hat A} \xrightarrow[\hat P_a|\psi\rangle]{a}$$

$p(a) = \langle\psi|\hat P_a|\psi\rangle$
(probability of measuring a. $\hat P_a$ does not have to be degenerate, could be tho.)

If $\hat P_a$ is degenerate, $p(a) = \sum_j |\langle a,j|\psi\rangle|^2$, $\hat P_a = \sum_j |a,j\rangle\langle a,j|$

CASE 2:

$$|\psi\rangle \longrightarrow \boxed{\hat B} \xrightarrow[\hat\Lambda_b|\psi\rangle]{b} \boxed{\hat A} \xrightarrow[\hat P_a \hat\Lambda_b|\psi\rangle]{a}$$

$p(a,b) = \|\hat P_a \hat\Lambda_b |\psi\rangle\|^2$
$= \langle\psi|\hat\Lambda_b^\dagger \hat P_a^\dagger \hat P_a \hat\Lambda_b|\psi\rangle$

(because $\hat P_a, \hat\Lambda_b$ are projectors) $= \langle\psi|\hat\Lambda_b \hat P_a \hat\Lambda_b|\psi\rangle$

In the very special case that $\hat A$ and $\hat B$ commute,

$p(a,b) = \langle\psi|\hat\Lambda_b \hat P_a \hat\Lambda_b|\psi\rangle = \langle\psi|\hat\Lambda_b \hat P_a|\psi\rangle = \langle\psi|\hat P_a \hat\Lambda_b|\psi\rangle$

CASE 3:

$$|\psi\rangle \longrightarrow \boxed{B} \xrightarrow[\hat\Lambda_b|\psi\rangle]{b} \boxed{A} \xrightarrow[\hat P_a \hat\Lambda_b|\psi\rangle]{a}$$

for <u>all</u> possible outcomes from measuring B

$p(a,b)$ is the same as case 2!

- What if we didn't know that we we measuring B in case 3, and could only see the result of measuring A?

$$p(a) = \underbrace{\sum_b p(a,b)}_{\text{from case 2}} = \sum_{b\in\sigma_B} \langle\Psi|\hat{\Lambda}_b \hat{P}_a \hat{\Lambda}_b|\Psi\rangle \neq \underbrace{\langle\Psi|\hat{P}_a|\Psi\rangle}_{\text{from case 1}}$$

<u>If</u> $\hat{A}$ and $\hat{B}$ commute, then:

$$\sum_{b\in\sigma_B} \langle\Psi|\hat{\Lambda}_b \hat{P}_a \hat{\Lambda}_b|\Psi\rangle = \sum_{b\in\sigma_B} \langle\Psi|\hat{\Lambda}_b \hat{P}_a|\Psi\rangle$$

$$= \langle\Psi|\underbrace{\Big(\sum_{b\in\sigma_B}\hat{\Lambda}_b\Big)}_{=\mathbb{I}}\hat{P}_a|\Psi\rangle = p(a) \text{ from case 1}$$

- So the <u>probability</u> of measuring a is the same as case 1 if $[\hat{A},\hat{B}]=0$ but the <u>state</u> is different!!

In case 1, state after final measurement is $\hat{P}_a|\Psi\rangle$

In case 3, there is no <u>definite</u> state (no single outcome):

$$\left.\begin{array}{l} \hat{P}_a\hat{\Lambda}_{b_1}|\Psi\rangle \\ \hat{P}_a\hat{\Lambda}_{b_2}|\Psi\rangle \\ \hat{P}_a\hat{\Lambda}_{b_3}|\Psi\rangle \\ \cdots \end{array}\right\} \text{an } \underline{\text{ensemble}} \text{ of states that occur with some probability.}$$

for all possible b, <u>even if</u> $[\hat{A},\hat{B}]=0$

→ Example ($\hat{A}$ and $\hat{B}$ commute)

Say $\hat{A}=\hat{L}_z$ and $\hat{B}=\hat{L}^2$ and we have a hydrogen atom prepared to be spin up, $n=3$, so $|n=3, \ell, m, \sigma=1/2\rangle = |\ell, m\rangle$.

$|\Psi\rangle = (|0,0\rangle + |1,0\rangle + |1,1\rangle + |2,0\rangle)\,1/2$

case 1:

$$|\Psi\rangle \longrightarrow \boxed{\hat{A}} \xrightarrow[\hat{P}_m|\Psi\rangle]{m} \begin{cases} m=0 & \hat{P}_0|\Psi\rangle = \frac{1}{2}(|0,0\rangle + |1,0\rangle + |2,0\rangle) = \frac{3}{4} \\ m=1 & \hat{P}_1|\Psi\rangle = \frac{1}{2}|1,1\rangle = \frac{1}{4} \\ \text{other } m & 0 \end{cases}$$

case 2:

$$|\Psi\rangle \longrightarrow \boxed{\hat{B}} \xrightarrow[\hat{\Lambda}_\ell|\Psi\rangle]{\ell} \begin{cases} \ell=0 & \hat{\Lambda}_0|\Psi\rangle = \frac{1}{2}|0,0\rangle = \frac{1}{4} \\ \ell=1 & \hat{\Lambda}_1|\Psi\rangle = \frac{1}{2}(|1,0\rangle + |1,1\rangle) = \frac{1}{2} \\ \ell=2 & \hat{\Lambda}_2|\Psi\rangle = \frac{1}{2}|2,0\rangle = \frac{1}{4} \end{cases}$$

- After measuring each possible ℓ in case 2, when we then measure m, you reproduce the probabilities from case 1:

$\ell : 0$ only state in $|\psi\rangle$ is $|0,0\rangle$, so $m = 0 \rightarrow P_{00} = \frac{1}{4}$

$\ell : 1$ can get $|1,0\rangle$ or $|1,1\rangle$ and $m = 0 \rightarrow P_{10} = \frac{1}{4}$

$m = 1 \rightarrow P_{11} = \frac{1}{4}$

$\ell : 2$ can get $|2,0\rangle$ so $m = 0 \longrightarrow P_{20} = \frac{1}{4}$

Overall, prob. of measuring $m = 0$ is still $\frac{3}{4}$ and of $m = 1$ is $\frac{1}{4}$!!

→ Example ($\hat{A}$ and $\hat{B}$ do not commute)

$\hat{A} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$ $\hat{B} = \begin{bmatrix} 3 & 1 \\ 1 & 4 \end{bmatrix}$

$\lambda = 1 : \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\mu =$

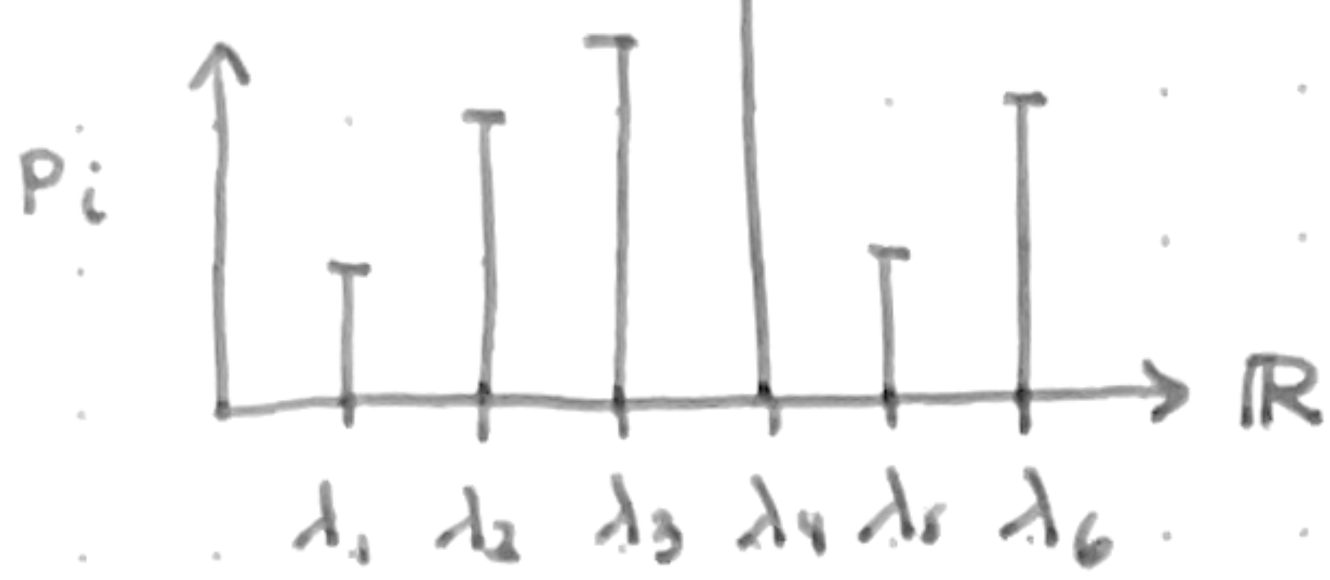
$\lambda = 2 : \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\mu =$

→ Incompatible Observables (continued)

- Initial state $|\psi\rangle = \sum_i c_i |i\rangle$ for eigenvectors $|i\rangle$ of $\hat{A} = \hat{A}^\dagger$.

(so as usual, $\langle i | j \rangle = \delta_{ij}$, $c_i = \langle i | \psi \rangle \to |\psi\rangle = \sum_i |i\rangle\langle i|\psi\rangle \ldots$)

$|\psi\rangle$ is a combination of states, so distribution of probabilities for each λ_i:



$$|\psi\rangle \longrightarrow \boxed{\hat{A}} \xrightarrow{\lambda_i}$$

$$p_i = |c_i|^2 = |\langle i | \psi \rangle|^2$$

p_i is $\| \hat{P}_{\lambda_i} |\psi\rangle \|^2$ and $\hat{P}_{\lambda_i} |\psi\rangle = |i\rangle\langle i| \left(\sum_i c_i |i\rangle\right)$

$$= c_i |i\rangle\langle i | i \rangle = c_i |i\rangle$$

$$= \langle c_i |i\rangle \,|\, c_i |i\rangle \rangle$$
$$= c_i^* c_i \langle i | i \rangle = |c_i|^2$$

- Standard deviation of $\hat{A}$, $\sigma_A = \sqrt{\sum_i p_i (\lambda_i - \bar{\lambda})^2}$

(normal definition)

By definition, $\bar{\lambda} = \langle \psi | \hat{A} | \psi \rangle$ and $p_i = |\langle i | \psi \rangle|^2$

$\langle \hat{A} \rangle = \sum_i p_i \lambda_i$ (by def. of expected value)

$$\langle \hat{A}^2 \rangle = \langle \psi | \hat{A}^2 | \psi \rangle = \sum_i \langle \psi \underbrace{| i \rangle \langle i |}_{= \mathbb{I} \text{ over all } i} \hat{A}^2 | \psi \rangle$$

$= \sum_i \langle \psi | i \rangle \langle i | \hat{A} \hat{A} | \psi \rangle$ and measuring $\hat{A}|\psi\rangle$ gives

$\hat{A}|\psi\rangle = \hat{A} \sum_i c_i |i\rangle = \sum_i c_i \hat{A} |i\rangle = \sum_i c_i \lambda_i |i\rangle$ and

$$\hat{A}\hat{A}|\psi\rangle = \sum_i c_i \lambda_i \hat{A} |i\rangle = \sum_i c_i \lambda_i^2 |i\rangle = |\psi\rangle \sum_i \lambda_i^2$$

Then $\langle \hat{A}^2 \rangle = \sum_i \langle \psi | i \rangle \langle i | \hat{A}^2 | \psi \rangle = \sum_i \langle \psi | i \rangle \langle i | \psi \rangle \lambda_i^2$

$$= \sum_i \lambda_i^2 |\langle i | \psi \rangle|^2 = \sum_i \lambda_i^2 p_i$$

$\langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle = \langle \hat{A}^2 - 2\hat{A}\langle \hat{A} \rangle + \langle \hat{A} \rangle^2 \rangle$ (normal FOIL)

$$= \langle \hat{A}^2 \rangle - 2\langle \hat{A} \rangle^2 + \langle \hat{A} \rangle^2 = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

$$\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2 = \sum_i \lambda_i^2 p_i - \langle \hat{A} \rangle^2$$

$$= \sum_i p_i (\lambda_i^2) - \langle \hat{A} \rangle^2 - 2\langle \hat{A} \rangle \sum_i p_i \lambda_i + 2\langle \hat{A} \rangle \sum_i p_i \lambda_i$$

$$= \sum_i p_i \lambda_i^2 + \langle \hat{A} \rangle^2 - 2\langle \hat{A} \rangle \sum_i p_i \lambda_i$$

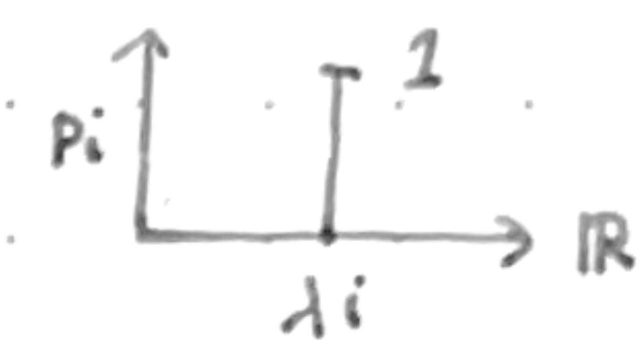
$$= \sum_i p_i \lambda_i^2 + \sum_i p_i \langle \hat{A} \rangle^2 - \sum_i 2\langle \hat{A} \rangle p_i \lambda_i$$

$$= \sum_i p_i \left(\lambda_i^2 + \langle \hat{A} \rangle^2 - 2\langle \hat{A} \rangle \lambda_i \right) = \sum_i p_i (\lambda_i - \langle \hat{A} \rangle)^2$$

So, $\langle \Psi | \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2 | \Psi \rangle = \sum_i p_i (\lambda_i - \bar{\lambda})^2$ (in full form)

$$\sigma_A = \sqrt{\textstyle\sum_i p_i (\lambda_i - \bar{\lambda})^2} = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

If $|\Psi\rangle$ is an eigenvector $|i\rangle$, then $\sigma_A = 0$,



- If $\hat{A}^\dagger = \hat{A}$, $\hat{B}^\dagger = \hat{B}$ and $[\hat{A}, \hat{B}] = 0$, $\hat{A}$ and $\hat{B}$ share a common basis of eigenvectors $|i\rangle$.
  - if $|\Psi\rangle = |i\rangle$, there's no uncertainty measuring $\hat{A}$ or $\hat{B}$. $\sigma_A = 0$, $\sigma_B = 0$
  - For any eigenstate of $\hat{A}$ (so $\sigma_A = 0$) you can find a vector in that eigenspace that is an eigenstate of $\hat{B}$.
- If $\hat{A}$ and $\hat{B}$ are incompatible ($[\hat{A}, \hat{B}] \neq 0$)...

→ Heisenberg uncertainty principle (theorem)

$$\sigma_A \sigma_B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|$$

Derivation:

- $|\phi_A\rangle \equiv (\hat{A} - \langle \hat{A} \rangle)|\Psi\rangle$ and $|\phi_B\rangle \equiv (\hat{B} - \langle \hat{B} \rangle)|\Psi\rangle$
- Schwarz inequality: $\forall |\Psi\rangle, |\phi\rangle$, $|\langle \Psi | \phi \rangle| \leq \| |\Psi\rangle \| \, \| |\phi\rangle \|$

We want to work from:

$$|\langle \phi_A | \phi_B \rangle| \leq \| |\phi_A\rangle \| \, \| |\phi_B\rangle \|$$

$$\| |\phi_A\rangle \|^2 = \langle \phi_A | \phi_A \rangle = \langle \Psi | (\hat{A} - \langle \hat{A} \rangle)^2 | \Psi \rangle = \sigma_A^2$$

and,

$$\| |\phi_B\rangle \|^2 = \sigma_B^2$$

- On the LHS: $\langle \phi_A | \phi_B \rangle = \langle \psi | (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) | \psi \rangle$
  call $\hat{A} - \langle \hat{A} \rangle = \Delta \hat{A}$ and $\hat{B} - \langle \hat{B} \rangle = \Delta \hat{B}$, so:

$$\langle \phi_A | \phi_B \rangle = \langle \psi | \Delta \hat{A} \Delta \hat{B} | \psi \rangle$$

$\Delta \hat{A} \Delta \hat{B}$ can be $\frac{1}{2}(\Delta \hat{A} \Delta \hat{B} + \Delta \hat{B} \Delta \hat{A}) + \frac{1}{2}\left(\frac{i}{i}\right)(\Delta \hat{A} \Delta \hat{B} - \Delta \hat{B} \Delta \hat{A})$
(just algebra)

each term is self-adjoint:

$$(\Delta \hat{A} \Delta \hat{B} + \Delta \hat{B} \Delta \hat{A})^\dagger = \Delta \hat{B}^\dagger \Delta \hat{A}^\dagger + \Delta \hat{A}^\dagger \Delta \hat{B}^\dagger$$
$$= \Delta \hat{B} \Delta \hat{A} + \Delta \hat{A} \Delta \hat{B}$$

etc.

$$\langle \phi_A | \phi_B \rangle = \underbrace{\frac{1}{2} \langle \psi | \{ \Delta \hat{A}, \Delta \hat{B} \} | \psi \rangle}_{\in \mathbb{R} \text{ bc self-adj}} + i/2 \underbrace{\langle \psi | \frac{[\Delta \hat{A}, \Delta \hat{B}]}{i} | \psi \rangle}_{\text{also } \in \mathbb{R}.}$$

$$|\langle \phi_A | \phi_B \rangle|^2 = \left| \frac{1}{2} \langle \psi | \{ \cdots \} | \psi \rangle + \frac{i}{2} \langle \psi | \frac{[\ldots]}{i} | \psi \rangle \right|^2$$

$$= \frac{1}{4} |\langle \psi | \{ \cdots \} | \psi |^2 + \frac{1}{4} |\langle \psi | [\cdots] | \psi \rangle|^2$$
$$\geq \frac{1}{4} |\langle \psi | [\cdots] | \psi \rangle|^2$$

$$\sigma_A^2 \sigma_B^2 \geq |\langle \phi_A | \phi_B \rangle|^2 \geq \frac{1}{4} |\langle \psi | [\cdots] | \psi \rangle|^2$$

$$\sigma_A^2 \sigma_B^2 \geq \frac{1}{4} |\langle \psi | [\Delta \hat{A}, \Delta \hat{B}] | \psi \rangle|^2$$

$$[\Delta \hat{A}, \Delta \hat{B}] = [\hat{A}, \hat{B}] - [\langle \hat{A} \rangle, \hat{B}] - [\hat{A}, \langle \hat{B} \rangle] + [\langle \hat{A} \rangle, \langle \hat{B} \rangle]$$
$$= [\hat{A}, \hat{B}]$$

$$\sigma_A \sigma_B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|$$

- Note if $\hat{A}$ and $\hat{B}$ do not commute, not <u>every</u> eigenstate $|\psi\rangle = |i\rangle$ gives uncertainty $= 0$ but <u>some</u> may.

e.g.

- $[\hat{x}, \hat{p}] = i\hbar$, $\sigma_x \sigma_p \geq \frac{1}{2} |\langle \psi | i\hbar | \psi \rangle| = \frac{\hbar}{2}$ so <u>no</u> state makes $\sigma_x = \sigma_p = 0$
- $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$ so not just some constant. $|l, m\rangle = |0, 0\rangle$ or an angular momentum of 0 yields $\sigma_{Lx} = \sigma_{Ly} = 0$, but you can't do this for <u>all</u> eigenvectors/values.

→ Unitary operators : $\hat{U}\hat{U}^{\dagger} = \hat{U}^{\dagger}\hat{U} = \mathbb{I}$

- $\hat{U}$ must be <u>invertible</u> and $\hat{U}^{-1} = \hat{U}^{\dagger}$
- Preserves inner product/norm:
  $\langle(\hat{U}\Psi)|(\hat{U}\Phi)\rangle = \langle\Psi|\hat{U}^{\dagger}\hat{U}|\Phi\rangle = \langle\Psi|\Phi\rangle$
- An <u>isometry</u> is a transformation that preserves scalar prod. (and norm, so angles and lengths are preserved).

<u>Not</u> all isometries are <u>invertible</u> so are not all unitary.
e.g. Shifting by 1 (add 1 to front)

$|1\rangle \rightarrow |2\rangle$. No $|\Psi\rangle$ exists so $\hat{A}|\Psi\rangle = |1\rangle$. Not surjective, so not invertible.

(Basically, unitary operators are surjective isometries...)