Week 8 - Unitary Operators, some asides

→ Determinants (an aside)

- The determinant has the following properties. It is:

1. Multilinear function of columns

   Say we have columns $\mathbb{a}, \mathbb{b}, \mathbb{c}, \dots$ in a matrix.

$$\det\left[\gamma \mathbb{a} + \beta \mathbb{b} \mid \mathbb{c} \mid \mathbb{d}\right]$$

$$= \alpha \det\left[\mathbb{a} \mid \mathbb{c} \mid \mathbb{d}\right] + \beta \det\left[\mathbb{b} \mid \mathbb{c} \mid \mathbb{d}\right]$$

2. Antisymmetric under a change of columns

$\det[\dots \mid \mathbb{a} \mid \dots \mid \mathbb{b} \mid \dots]$ where $\mathbb{a}$ is the i^{th} column, $\mathbb{b}$ is the j^{th} column

$= -\det[\dots \mid \mathbb{b} \mid \dots \mid \mathbb{a} \mid \dots]$ where indices of $\mathbb{a}$ and $\mathbb{b}$ are flipped.

3. One on $\mathbb{1}$

$$\det(\mathbb{1}) = \det(\mathbb{I}) = 1$$

- linearly dependent columns ⟺ determinant $= 0$

  Say we have a matrix $\mathbb{C}$ with columns $\mathbb{C}^i$ where:

  $\sum_{i=1}^{n} \mathbb{C}^i \alpha_i = 0$ and not all $\alpha_i = 0$. The columns are linearly dependent.

  Then, the first column, $\mathbb{C}^1 = -\frac{1}{\alpha_1} \sum_{i=2}^{n} \mathbb{C}^i \alpha_i$ (pull out 1st term from summation.)

$$\det(\mathbb{C}) = \det\left[\sum_{i=2}^{n} \frac{\alpha_i}{\alpha_1} \mathbb{C}^i \mid \mathbb{C}^2 \mid \dots\right]$$

  according to property #1 we can pull out constants and separate terms:

$$\det(\mathbb{C}) = \frac{\alpha_2}{\alpha_1} \det\left[\underline{\mathbb{C}^2} \mid \underline{\mathbb{C}^2} \mid \dots\right] + \frac{\alpha_3}{\alpha_1} \det\left[\underline{\mathbb{C}^3} \mid \mathbb{C}^2 \mid \underline{\mathbb{C}^3} \mid \dots\right]$$

  each term has a repeat column!

  By property #2 we know $\det[\dots \mid \mathbb{a} \mid \dots \mid \mathbb{a} \mid \dots]$ is equal to $-\det[\dots \mid \mathbb{a} \mid \dots \mid \mathbb{a} \mid \dots]$ (swapping columns), so the determinant of each term is 0.

  So, $\det(\mathbb{C}) = 0$.

→ More on unitary operators

- We know $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \mathbb{I} \Leftrightarrow \hat{U}$ are surjective isometries
- Given basis $\{|\phi_i\rangle\}_{i=1,\dots,n}$ and $\langle\phi_i|\phi_j\rangle = \delta_{ij}$ then $\{\hat{U}|\phi_i\rangle\}_{i=1,\dots,n}$ is also a basis.

(this is true in infinite dimensional spaces also since $\hat{U}$ is surjective)

- If we have two ONB $\{|v_i\rangle\}$ and $\{|u_i\rangle\}$, we can find:

$$\hat{U}|u_i\rangle = |v_i\rangle \quad \forall i \in I$$

$$\hat{U} = \sum_{i=1}^{n} |v_i\rangle\langle u_i|$$

$$\hat{U}|u_j\rangle = \sum_{i=1}^{n} |v_i\rangle\langle u_i|u_j\rangle = \sum_{i=1}^{n} |v_i\rangle\delta_{ij} = |v_j\rangle$$

- $\hat{U}$ and $\hat{U}^\dagger$ commute.

For any operator we can write: $\hat{U} = \frac{\hat{U}+\hat{U}^\dagger}{2} + i\,\frac{\hat{U}-\hat{U}^\dagger}{2i}$

where $\hat{X} = \frac{\hat{U}+\hat{U}^\dagger}{2}$, $\hat{Y} = \frac{\hat{U}-\hat{U}^\dagger}{2i}$. We know $\hat{X}$ and $\hat{Y}$ are self-adjoint:

$$\hat{X}^\dagger = \frac{1}{2}(\hat{U}+\hat{U}^\dagger)^\dagger = \frac{1}{2}(\hat{U}^\dagger+\hat{U}) = \hat{X}, \text{ etc.}$$

In <u>this</u> case, since $\hat{U}$ and $\hat{U}^\dagger$ commute, $\hat{X}$ and $\hat{Y}$ commute. That means there is a <u>common basis of eigenvectors</u> between $\hat{X}$ and $\hat{Y}$:

$$\hat{X}|\lambda,\mu,i\rangle = \lambda|\lambda,\mu,i\rangle \text{ and } \hat{Y}|\lambda,\mu,i\rangle = \mu|\lambda,\mu,i\rangle$$

then:

$$\hat{U}|\lambda,\mu,i\rangle = (\lambda+i\mu)|\lambda,\mu,i\rangle$$

so, $\hat{U}$ must have <u>complex</u> eigenvalues.

(also, $\langle\lambda,\mu,i|\lambda',\mu',j\rangle = \delta_{\lambda\lambda'}\delta_{\mu\mu'}\delta_{ij}\dots$)

- If $\hat{U}|\lambda\rangle = \lambda|\lambda\rangle$:

$$\|\hat{U}|\lambda\rangle\|^2 = \langle\hat{U}\lambda|\hat{U}\lambda\rangle = \langle\lambda|\hat{U}^\dagger\hat{U}|\lambda\rangle = \langle\lambda|\lambda\rangle$$

$$= |\lambda|^2\langle\lambda|\lambda\rangle = \langle\lambda|\lambda\rangle$$

$$|\lambda|^2 = 1$$

so, $\lambda = 1\cdot e^{i\theta}$

→ Phase factors (another aside)

ONB $\{|1\rangle, |2\rangle, |3\rangle\}$ means $\{|1\rangle i, |2\rangle e^{i\pi/3}, |3\rangle(-1)\}$ is still an ONB. Magnitude $||i\rangle|^2$ is still 1, direction doesn't change.

→ Unitary operators and self-adjoint operators

- If $\hat{A} = \hat{A}^\dagger$, there is a $\hat{u} = e^{-i\hat{A}}$ that is unitary. (negative sign by convention)

proof ver. 1:

$$\hat{u}^\dagger = e^{i\hat{A}^\dagger}, \quad \hat{u}\hat{u}^\dagger = \hat{u}^\dagger\hat{u} = e^{i\hat{A}}e^{-i\hat{A}} = \hat{1}$$

proof ver. 2:

By spectral thm: $\hat{A} = \sum_{\lambda \in \sigma(A)} \lambda \hat{P}_\lambda$ so $f(\hat{A}) = \sum_\lambda f(\lambda)\hat{P}_\lambda$

that means $\hat{u} = \sum_{\lambda \in \sigma(A)} e^{-i\lambda}\hat{P}_\lambda$ and $\hat{u}^\dagger = \sum_{\lambda \in \sigma(A)} e^{i\lambda}\hat{P}_\lambda$

so $$\hat{u}\hat{u}^\dagger = \sum_\lambda e^{-i\lambda}\hat{P}_\lambda \sum_{\lambda'} e^{i\lambda'}\hat{P}_{\lambda'}$$

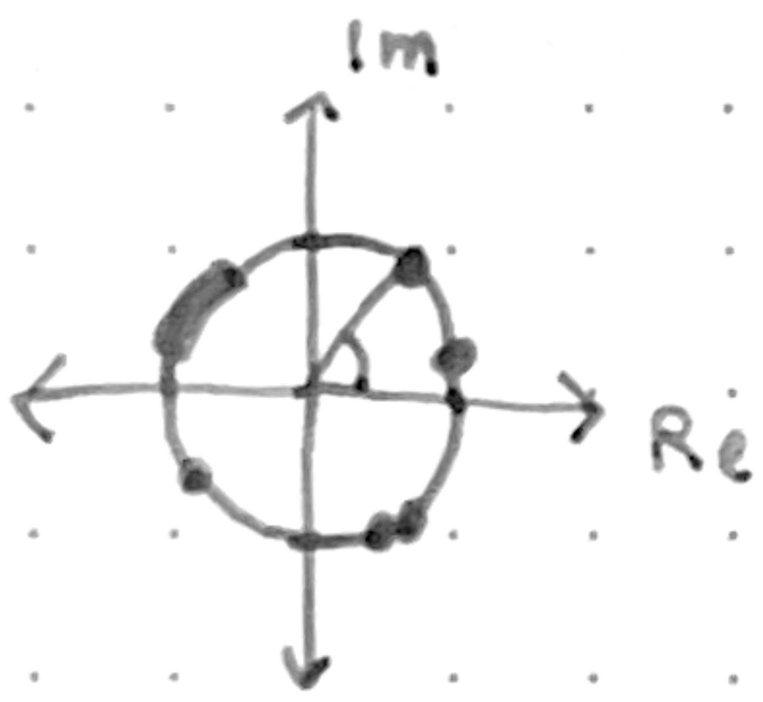
$$= \sum_{\lambda,\lambda'} e^{-i\lambda} e^{i\lambda'} \hat{P}_\lambda \hat{P}_{\lambda'} = \sum_{\lambda,\lambda'} e^{i(\lambda'-\lambda)} \underbrace{\delta_{\lambda\lambda'}\hat{P}_\lambda}_{\hat{P} \text{ are idempotent}}$$

$$= \sum_\lambda \hat{P}_\lambda = \hat{1}$$

- The opposite is also true: if $\hat{u}$ is unitary, there is an $\hat{A} = \hat{A}^\dagger$ so $\hat{u} = e^{-i\hat{A}}$ (there can be more than one possible $\hat{A}$ ...)

proof:

$\hat{u}|\lambda, i\rangle = \lambda|\lambda, i\rangle$, we know $\lambda \in \mathbb{C}$ and $|\lambda| = 1$ so we can visualize λ as:



So a λ can be ^(uniquely!) defined as θ_λ from the real axis: $\lambda = e^{i\theta_\lambda}$, $\theta_\lambda \in (-\pi, \pi]$

Because $\hat{u}$ is diagonalizable:

$$\hat{u} = \sum_{\lambda \in \sigma} \lambda \hat{P}_\lambda = \sum_\lambda e^{i\theta_\lambda}\hat{P}_\lambda \rightarrow \hat{A} = -\sum_{\lambda \in \sigma(u)} \theta_\lambda \hat{P}_\lambda$$

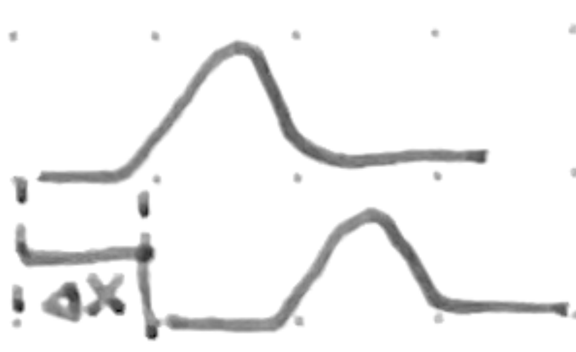
$\hat{A}$ can be spectrally defined, so it is self-adjoint.

→ Families of unitary operators

- Often times you don't just have a $\hat{u}$, you have a $\hat{u}(t)$ where each unique input parameter may yield a unique operator.

e.g. translations:

- $\hat{T}_{\Delta x}\,\psi(x)$ that shifts $\psi(x)$ by Δx: is parameterized by Δx



- This family has members $\hat{U}(t) = e^{-i\hat{A}t}$, $\hat{A} = \hat{A}^{\dagger}$ $t \in \mathbb{R}$ so infinitely many $\hat{U}(t)$'s.

These families are <u>abelian groups</u>:

- $\hat{U}(0) = e^{0} = \hat{1}$ so contains the <u>identity</u>
- $\hat{U}(t)\,\hat{U}(t')$ as a composition is $e^{-i\hat{A}t}\, e^{-i\hat{A}t'} = e^{-iA(t+t')}$ $= \hat{U}(t+t')$, so we can say there is <u>associativity</u>
- $\hat{U}(-t) = e^{i\hat{A}t} = \hat{U}^{\dagger}(t) = (\hat{U}(t))^{-1}$ so there is a <u>symmetric element</u>
- For an arbitrary $\hat{U}(t)$ and $\hat{U}(t')$, $\hat{U}(t)\hat{U}(t') = \hat{U}(t')\hat{U}(t)$, so there is <u>commutativity</u>.

We can also show $\forall |\Psi\rangle \in H, \lim_{t \to 0} \| \hat{U}(t)|\Psi\rangle - |\Psi\rangle \| = 0$ (he didn't tho)

which means it is a <u>strongly continuous</u> group.

$\hat{A} = i\, {}^{d}/_{dt}\, \hat{U}(t)|_{t=0}$

→ Stone Theorem

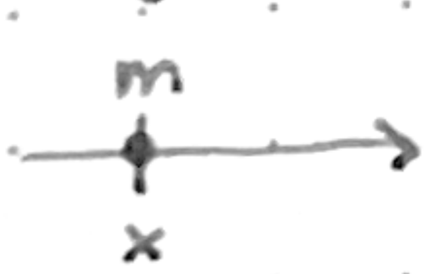
- For a strongly continuous, one-parameter group of unitary transformations: $\exists!\ \underbrace{\hat{A} = \hat{A}^{\dagger}}_{\text{observable}} \mid \underbrace{\hat{U}(t) = e^{-i\hat{A}t}}_{\text{continuous symmetries}}$

($\hat{U}(t)$ is similar to the classical canonical transformations)

This tells us that each unitary transformation $\hat{U}(t)$ <u>can</u> be directly determined by observable $\hat{A}$. Sometimes it's not so simple...

→ The bridge between classical and quantum mechanics

- If we have a particle moving in 1D:



  - $x \in \mathbb{R}$, we can measure position / x
  - Must be a corresponding $\hat{X} = \hat{X}^{\dagger}$

- $\hat{X}$ is covered under the spectral theorem:

  $\hat{X}|x\rangle = x|x\rangle$ for all possible measurements x, so $\sigma(\hat{X}) \in \mathbb{R}$

- This raises two issues:
  1. The spectrum of $\hat{X}$ is <u>continuous</u>!
  2. " " " " is <u>not bounded</u>!

→ Issues with #1

- We can't just say $\sum_x |x\rangle\langle x| = \hat{1}$ because there is no discrete x.

  Instead: $\hat{1} = \int dx\, |x\rangle\langle x|$ and $|x\rangle\langle x|$ is a <u>projector density</u>

(basically, $|x\rangle\langle x| = \frac{d\hat{P}}{dx}$ instead of just $\hat{P}$. small $d\hat{P}$ over dx is a density...)

Then:

$|\Psi\rangle = \hat{1}|\Psi\rangle = \int dx\, |x\rangle\langle x|\Psi\rangle$

and $\langle x|\Psi\rangle$ is equivalent to the $\Psi(x)$ position-space wave-function.

($|\langle x|\Psi\rangle|^2$ is the probability density of finding the system in or near? position x <u>specifically</u>)

$$\langle x|\Psi\rangle = \langle x|\underbrace{\int dx'\, |x'\rangle\langle x'|}_{\text{identity}}\Psi\rangle = \int dx'\, \langle x|x'\rangle\langle x'|\Psi\rangle$$

$$= \int dx'\, \delta(x-x')\langle x'|\Psi\rangle$$

which means that $|x\rangle$ is not normalizable! $\langle x|x'\rangle \Rightarrow \langle x|x\rangle = \delta(0)$ which is ∞, and <u>can't</u> be 1.

- $|x\rangle$ here is <u>not</u> a state of a quantum system, it is a <u>generalized eigenstate</u>.

  Not quite a function but a distribution that acts on a function?

→ Issues with #2

- The Hellinger-Toeplitz Theorem says if an operator $\hat{A}$ is defined on the whole Hilbert space, it is bounded:

  supremum/least upper bound of $\|\hat{A}|\Psi\rangle\| < \infty$, $|\Psi\rangle \in H$ and $\||\Psi\rangle\| = 1$

- We know that $\hat{X}$ is not bounded, meaning it is <u>not</u> defined on the whole Hilbert Space!

This means such an operator has a non-trivial domain:

- For a single $|\Psi\rangle$, $\langle\Psi|\Psi\rangle < \infty$ for sure. Then,

  $\langle\Psi|\hat{1}|\Psi\rangle = \langle\Psi|\int dx\, |x\rangle\langle x|\Psi\rangle = \int dx\, \langle\Psi|x\rangle\langle x|\Psi\rangle$

  $= \int dx\, |\Psi(x)|^2 < \infty$

  so, $\Psi(x) \in L^2(\mathbb{R})$.

- That means $|\Psi\rangle \mapsto \langle x|\Psi\rangle$ maps $H \to L^2(\mathbb{R})$

- Now, $\langle x|\hat{X}|\Psi\rangle$ means we measure position for $|\Psi\rangle$ and project into position space (?)

$$\langle x|\hat{X}|\Psi\rangle = \langle x|\hat{X}\int dx'\, |x'\rangle\langle x'|\Psi\rangle = \int dx'\, \langle x|\hat{X}|x'\rangle\Psi(x')$$

$$= \int \langle x|\,(x'|x'\rangle)\Psi(x')\,dx' = \int dx'\, x'\,\delta(x-x')\,\Psi(x')$$

$$= x\,\Psi(x).$$ Is this still in $L^2(\mathbb{R})$?

Say that $\Psi(x) = \frac{1}{\sqrt{(1+x^2)\pi}}$. Then:

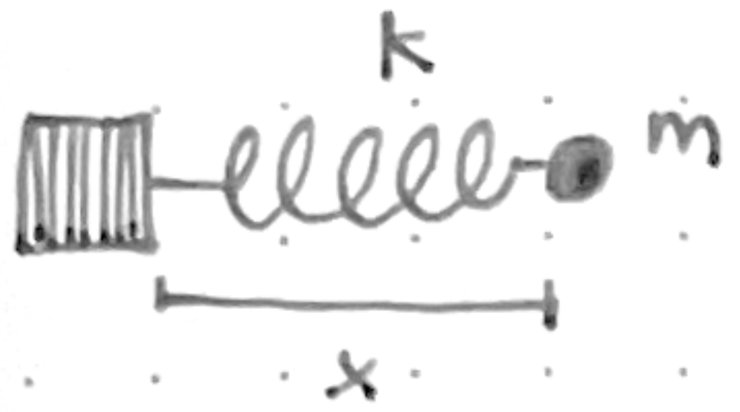
$$\int_{-\infty}^{\infty} dx\, |\Psi(x)|^2 = \frac{1}{\pi}\int_{-\infty}^{\infty} dx\, \frac{1}{1+x^2} = 1$$

what about $x\Psi(x)$?

$$\int_{-\infty}^{\infty} dx\, \frac{1}{\pi}\frac{x^2}{1+x^2} = \infty$$

This means that $\hat{X}$ acts on $\Psi(x)$ and gives a vector $x\Psi(x)$ with infinite length, so this particular $\Psi(x)$ is not in the domain of the operator $\hat{X}$: It's position is undefined!!

→ Classical mechanics



$$T(q,\dot{q}) = \frac{1}{2}m\dot{x}^2 \qquad p = m\dot{x}$$
$$V(q) = \frac{1}{2}kx^2$$

$$L(q,\dot{q}) = T(q,\dot{q}) - V(q) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$$

$$p(q,\dot{q}) = \frac{\partial L}{\partial \dot{q}} \quad \text{(canonically conjugated momentum)}$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q} \rightarrow m\ddot{x} = -kx \quad \text{(Hook's law, N2L!)}$$

Then also: $\dot{x} = p/m$

$$\underbrace{H(q,p) = p\dot{q}(q,p) - L(q,p)}_{\text{Legendre Transform}} = \frac{p^2}{m} - \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2$$
$$= \frac{p^2}{2m} + \frac{1}{2}kx^2$$

In this case, this is the energy of the system.

$$\dot{p} = -\frac{\partial H}{\partial q} \text{ and } \dot{q} = +\frac{\partial H}{\partial p} \rightarrow \dot{x} = \frac{p}{m} \text{ and } \dot{p} = -kx \text{ again.}$$