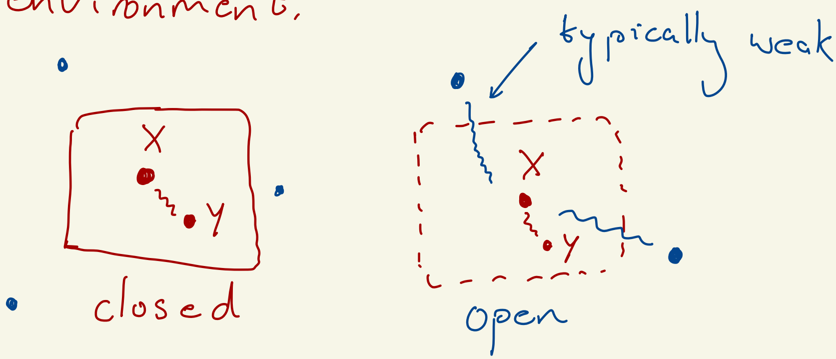
Postulate 2: The evolution of a closed* quantum system is described by a unitary transformation. Specifically, the state $|\psi\rangle$ of the system at time t_1 is related to the state $|\psi'\rangle$ at t_2 by a unitary operator U which depends only on t_1 & t_2.

$$\rightsquigarrow \quad |\psi(t_2)\rangle = \underset{t_1 \longrightarrow t_2}{U(t_1, t_2)}\, |\psi(t_1)\rangle$$

* NB: The assumption of a closed quantum system is a simplification. In general quantum systems will interact with their environment.



We can write down a refined version of postulate 2...

Postulate 2*: The time evolution of the state of a closed quantum system is described by the Schrödinger equation...

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle \quad \text{SE}$$

where

- $\hbar$ is Planck's constant (normally set $\hbar = 1$)
- H is a Hermitian operator called the system Hamiltonian.

→ If we know the Hamiltonian & initial state $|\psi(0)\rangle$ we can solve SE to find $|\psi(t)\rangle$ for all t.

We can now obtain postulate 2 from postulate 2*... 4

↳ for simplicity we assume H is time independent...

↳ In this case we can solve SE to obtain

$\hbar = 1$

$$|\psi(t_2)\rangle = e^{-iH(t_2-t_1)} |\psi(t_1)\rangle$$

$$= U(t_1, t_2) |\psi(t_1)\rangle$$

$$\boxed{\text{Crux: } U(t_1,t_2) = \underbrace{e^{-iH(t_2-t_1)}}_{\text{Matrix exponential!}}}$$

Excercises

1. Prove $U(t_1, t_2)$ is unitary.
2. Write down an expression for $U(t_1, t_2)$ when $H = H(t)$ is time dependent.

Matrix exponential

$$e^X := \sum_{k=0}^{\infty} \frac{1}{k!} X^k$$ Definition

Properties

- $e^0 = \mathbb{1}$
- $e^{X^T} = (e^X)^T$
- if Y is invertible $e^{YXY^{-1}} = Y e^X Y^{-1}$
- $[X,Y] = 0 \implies e^{X+Y} = e^X e^Y$

DANGER! $\underbrace{[X,Y]}_{\text{commutator!}} \neq 0 \xrightarrow[\text{be}]{\text{can}} e^{X+Y} \neq e^X e^Y$

- $[X,Y] = XY - YX$
- $\{X,Y\} = XY + YX$ → anti-commutator

Terminology

↳ if $[X, Y] = 0$ we say X & Y commute

↳ $XY = YX$ ⟹ order of application doesn't matter.

→ if $\{X, Y\} = 0$ we say X & Y anti-commute.

Before moving on let's check our soln to (SE)

↳ Claim: $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ is soln to (SE)

$\hbar = 1$

Proof: $$i\frac{d|\psi(t)\rangle}{dt} = i\,d/dt\left(e^{-iHt}|\psi(0)\rangle\right)$$

$$= i(-iH)\underbrace{\left[e^{-iHt}|\psi(0)\rangle\right]}_{|\psi(t)\rangle}$$

$$= H|\psi(t)\rangle$$

∎

Note:

1. For all Hermitian operators H & $\forall\, t \geq 0$ the operator

$$U(t) = e^{-iHt}$$

is unitary.

2. For all unitary operators $U(t)$ there exists some Hermitian operator H such that

$$U(t) = e^{-iH(t)}$$

*

Crux: We can think of all unitary evolutions as arising from evolution under some Hamiltonian H

↳ Designing quantum gates means engineering system Hamiltonians!

* Think about group $SU(n)$ with lie-algebra $su(n)$

NB → Figuring out the Hamiltonian of a system, or designing a system with a specific Hamiltonian, is not easy!

→ Requires intuition + experiments!

Examples

- magnet
- molecule
- laser
- superconductor
- photosynthetic complex

Guess + experiment!

Developing methods to learn Hamiltonians from system measurements is an active field!

Recall that the Hamiltonian H is a Hermitian operator...

↳ ∴ we can write

normalized eigenvector

$$H = \sum_i E_i |E_i\rangle\langle E_i|$$

real eigenvalues

↳ $\boxed{\text{NB}}$ $H|E_i\rangle = E_i |E_i\rangle$

We call $|E_i\rangle$ a stationary state:

↳ set $|\psi(0)\rangle = |E_i\rangle$...

$$|\psi(t)\rangle = e^{-iHt}|E_i\rangle$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} (-i)^k H^k |E_i\rangle$$

$$= \sum_k \frac{1}{k!} (-i)^k E_i^k |E_i\rangle$$

$$= e^{-iE_i t} |E_i\rangle$$

↳ Global phase - cannot be observed!

Observables

↳ In quantum mechanics observables are described by Hermitian matrices acting on the state space of the system.

⟹ Given a Hermitian operator O we can always write

$$O = \sum_m E_m \underbrace{|E_m\rangle\langle E_m|}_{\text{↳ projector onto } m\text{'th eigenspace}}$$

$$= \sum_m E_m P_m$$

where $\{P_m\}$ is a valid projective measurement.

By "measure O" we mean "do the projective measurement $\{P_m\}$".

↳ get eigenvalue E_m with prob $\| P_m |\psi\rangle \|^2$

We often set $E_m = m \Rightarrow O = \sum_m m P_m$

We will often care about the average value when measuring $\mathcal{O}$. (12)

call it <u>expectation value of $\mathcal{O}$</u>. $\underset{\shortparallel}{E(\mathcal{O})}$

$$E(\mathcal{O}) = \sum_m m\, p(m)$$

$$\mathcal{O} = \sum_m m P_m = \sum_m m |E_m\rangle\langle E_m|$$

$$= \sum_m m \langle\psi|P_m|\psi\rangle$$

$$= \langle\psi| \sum_m m P_m |\psi\rangle$$

$$= \langle\psi|\mathcal{O}|\psi\rangle$$

$$\boxed{E(\mathcal{O}) = \langle\psi|\mathcal{O}|\psi\rangle := \langle\mathcal{O}\rangle}$$

We also care about the standard deviation...

$$[\Delta(\mathcal{O})]^2 = \langle(\mathcal{O} - \langle\mathcal{O}\rangle)^2\rangle$$

$$= \langle\mathcal{O}^2\rangle - \langle\mathcal{O}\rangle^2$$

Exercise: Suppose we have an observable O & $|\psi\rangle$ is an eigenstate of O with eigenvalue m. What is $\langle O \rangle$ & $\Delta(O)$ when measuring $|\psi\rangle$?

Example: $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$= 1 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - 1 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= 1 P_1 + (-1) P_{-1}$$

"Measure Z" means do the projective measurement $\{P_1, P_{-1}\}$

Note: $P_1 |1\rangle = 0 \qquad P_1 |0\rangle = |0\rangle$

$P_{-1} |1\rangle = |1\rangle \qquad P_{-1} |0\rangle = 0$

if $|\psi\rangle = |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$

$$\langle Z \rangle = \langle \psi | Z | \psi \rangle$$

$$= \tfrac{1}{\sqrt{2}} (\langle 0| + \langle 1|)(|0\rangle + |1\rangle) \tfrac{1}{\sqrt{2}}$$

$$= \tfrac{1}{2} \langle 0|0\rangle - \tfrac{1}{2} \langle 1|1\rangle$$

$$= \underline{0}$$

Let's go back to Hamiltonians...

↳ Hamiltonians are Hermitian

↳ ∴ They are observables!

$$H = \sum_i E_i \underbrace{\overbrace{|E_i\rangle\langle E_i|}^{P_i}}$$

↳ stationary state or energy eigenstate

when we measure H we get E_i with $p(E_i) = ||\langle E_i|\psi\rangle||^2$

↳ The smallest result we can get is

$$E_g = \min_i (E_i)$$

↳ ground state energy!

↳ at 0K the system will be in $|E_g\rangle$

∴ Physically very relevant!!