Quantum Mechanics & Quantum Computation

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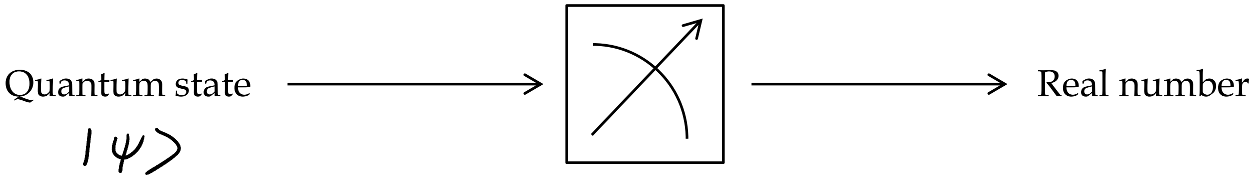
Lecture 12: Observables and Schrödinger's equation

Observables (part 1)

Observable

- An **observable** is a quantity like energy, position, momentum



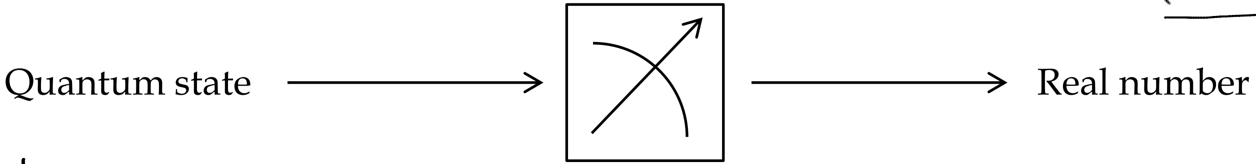
Observable

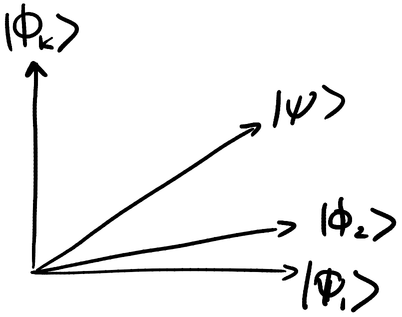
- Suppose we have a k-level system: $|\psi\rangle \in \mathbb{C}^k$

- An observable A for this system is an operator: a kxk Hermitian matrix.

$$A = A^\dagger$$

e.g. $\begin{pmatrix} 1 & 1+i \\ 1-i & -2 \end{pmatrix}$





outcome j w.p. $|\alpha_j|^2$ new state is $|\phi_j\rangle$

Observable

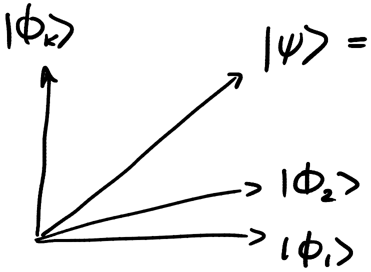
- An observable A for a k-level system is an operator: a kxk Hermitian matrix.

$$A = A^\dagger \qquad \text{e.g.} \begin{pmatrix} 1 & 1+i \\ 1-i & -2 \end{pmatrix}$$

<u>What's special Hermitian matrices?</u> **Spectral theorem!**

A has orthonormal eigenvectors $|\phi_1\rangle, \ldots, |\phi_k\rangle$ with real eigenvalues $\lambda_1, \ldots, \lambda_k$

$$A|\phi_i\rangle = \lambda_i|\phi_i\rangle$$



$|\psi\rangle = \alpha_1|\phi_1\rangle + \cdots + \alpha_k|\phi_k\rangle$

with prob. $|\alpha_j|^2$ outcome is λ_j

new state is $|\phi_j\rangle$

- Example $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$.
- Observable $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = -\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

evectors : $|+\rangle$, $|-\rangle$

evalues : 1 $\quad -1$

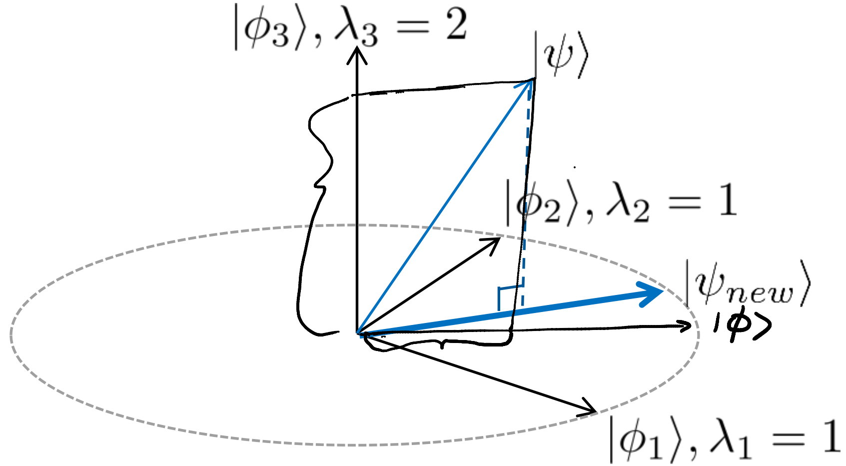
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \frac{\alpha+\beta}{\sqrt{2}}|+\rangle + \frac{\alpha-\beta}{\sqrt{2}}|-\rangle$$

1 w.p. $\left|\frac{\alpha+\beta}{\sqrt{2}}\right|^2$ new state $= |+\rangle$

-1 wp $\left|\frac{\alpha-\beta}{\sqrt{2}}\right|^2$ new state $= |-\rangle$

Expected outcome $= 1 \cdot \left|\frac{\alpha+\beta}{\sqrt{2}}\right|^2 + -1 \cdot \left|\frac{\alpha-\beta}{\sqrt{2}}\right|^2$

- Repeated eigenvalues?



What happens if the measurement outcome is 1?

$|\phi\rangle = \alpha|\phi_1\rangle + \beta|\phi_2\rangle$

Does it collapse to $|\phi_1\rangle$ or $|\phi_2\rangle$?

$A|\phi\rangle = \alpha A|\phi_1\rangle + \beta A|\phi_2\rangle$

$= \alpha \cdot 1 |\phi_1\rangle + \beta \cdot 1 |\phi_2\rangle$

It gets projected into the eigenspace.

$= \alpha|\phi_1\rangle + \beta|\phi_2\rangle = |\phi\rangle$

- What happens if we measure a quantum system with respect to the observable I?

$$I = \begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & \ddots & \\ 0 & & & 1 \end{bmatrix}$$

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Lecture 12: Observables and Schrödinger's equation

Observables (part 2)

Observable

- An observable A for a k-level system is an operator: a kxk Hermitian matrix.

$$A = A^\dagger \qquad\qquad \text{e.g.} \begin{pmatrix} 1 & 1+i \\ 1-i & -2 \end{pmatrix}$$

- Measure in eigenbasis:

A has orthonormal eigenvectors $|\phi_1\rangle, \ldots, |\phi_k\rangle$ with real eigenvalues $\lambda_1, \ldots, \lambda_k$

$$A|\phi_i\rangle = \lambda_i|\phi_i\rangle$$

- How general is this?

- Suppose we wish to measure in an arbitrary basis $|\phi_1\rangle, \ldots, |\phi_k\rangle$
  and want arbitrary real outcomes $\lambda_1, \ldots, \lambda_k$
  is there an observable A with corresponding eigenvectors and eigenvalues?

<u>Example</u>: $|\phi_1\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{i}{\sqrt{2}}|1\rangle$ $\qquad$ $|\phi_2\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{i}{\sqrt{2}}|1\rangle$

$\lambda_1 = +1$ $\qquad$ $\lambda_2 = -1$.

A

$|\phi\rangle$ project onto $|\phi\rangle$ $\quad$ $\underline{\underline{P}}$

$P = |\phi\rangle\langle\phi|$. $\qquad$ $P|\psi\rangle = |\phi\rangle\underbrace{\langle\phi||\psi\rangle} = \underbrace{\langle\phi|\psi\rangle}|\phi\rangle$

$$A = 1\cdot|\phi_1\rangle\langle\phi_1| + (-1)|\phi_2\rangle\langle\phi_2|$$

$$|\phi_1\rangle\langle\phi_1| = \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & 1/2 \end{pmatrix}$$

$$|\phi_2\rangle\langle\phi_2| = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -i/\sqrt{2} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} & i/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 1/2 & i/2 \\ -i/2 & 1/2 \end{pmatrix}$$

$$A = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} \\ -i/\sqrt{2} \end{pmatrix} = \begin{pmatrix} -1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} = -1\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix}$$

$$A|\phi_1\rangle$$
$$= (|\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2|)|\phi_1\rangle$$
$$= |\phi_1\rangle\underbrace{\langle\phi_1|\phi_1\rangle}_{1} - |\phi_2\rangle\underbrace{\langle\phi_2|\phi_1\rangle}_{\overset{!}{0}}$$
$$= |\phi_1\rangle - 0 = |\phi_1\rangle$$

$$A|\phi_2\rangle = -|\phi_2\rangle$$

- In general: Given $\underline{\underline{|\phi_i\rangle}}, \underline{\underline{\lambda_i}}$ corresponding observable is:

$$A = \sum \underline{\underline{\lambda_i}} \underbrace{|\phi_i\rangle\langle\phi_i|}_{P_i}$$

$|\phi_j\rangle$ evectr $\quad A|\phi_j\rangle = \sum \lambda_i P_i |\phi_j\rangle$

$$= \underline{\underline{\lambda_j}} |\phi_j\rangle$$

orthonormal basis $\longleftrightarrow$ observable.

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Lecture 12: Observables and Schrödinger’s equation

Schrödinger’s equation (part 1)

Axiom of unitary evolution

- **Unitary evolution axiom**: a quantum system evolves by a unitary rotation of the Hilbert space.

$$UU^\dagger = U^\dagger U = I$$

- But… by *which* unitary rotation?

This is described by **Schrödinger's equation,**
"the quantum equation of motion"

Schrödinger's equation

- Energy observable H, called the Hamiltonian of the system.
  - Its eigenvectors $|\phi_i\rangle$'s are the states with definite energy.
  - The eigenvalues λ_i's are the energy of the corresponding state.

- Example $H = \begin{pmatrix} -\frac{1}{2} & \frac{5}{2} \\ \frac{5}{2} & -\frac{1}{2} \end{pmatrix}$
  - $|+\rangle$ with energy = 2
  - $|-\rangle$ with energy = -3

$|\psi\rangle = |+\rangle$

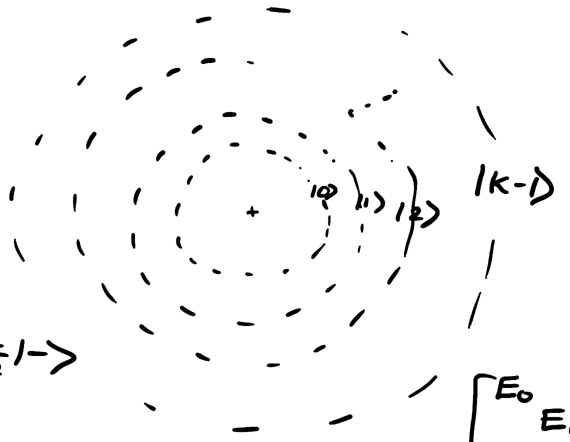
$|\psi\rangle = |-\rangle$

$|\psi\rangle = |0\rangle$

$= \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}|-\rangle$

2 wp $\frac{1}{2}$

-3 wp $\frac{1}{2}$.



$$H = \begin{bmatrix} E_0 & & & 0 \\ & E_1 & & \\ & & \ddots & \\ 0 & & & E_{k-1} \end{bmatrix}$$

Schrödinger's equation

- Schrödinger's equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

Given $|\psi(0)\rangle$, H figure out $|\psi(t)\rangle$

$i = \sqrt{-1}$

$\hbar$ reduced Planck constant $\hbar = \frac{h}{2\pi}$

Planck relation $\underline{\underline{E}} = h\,\underline{\underline{\nu}}$

$$\boxed{\begin{aligned} h &= 6.26 \times 10^{-34}\ \mathrm{Js} \\ \hbar &= 1.055 \times 10^{-34}\ \mathrm{Js} \\ &= 6.58 \times 10^{-16}\ \mathrm{eV\cdot s} \end{aligned}}$$

Solving Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

$|\psi(0)\rangle = |\phi_j\rangle$ where $|\phi_j\rangle$ is some eigenvector of H with a corresponding eigenvalue $|\lambda_j\rangle$

Then $|\psi(t)\rangle = e^{-\frac{i\lambda_j t}{\hbar}}|\phi_j\rangle$ rate of precession $\propto$ energy.

$$H|\phi_j\rangle = \lambda_j|\phi_j\rangle \Rightarrow |\psi(t)\rangle = a(t)|\phi_j\rangle \longrightarrow |\phi_j\rangle$$

$$i\hbar\frac{\partial}{\partial t}(a(t)|\phi_j\rangle) = H\,a(t)|\phi_j\rangle$$

$$\left[i\hbar\frac{\partial}{\partial t}a(t)\right]|\phi_j\rangle = a(t)\lambda_j|\phi_j\rangle$$

$$i\hbar\frac{\partial a(t)}{\partial t} = a(t)\lambda_j$$

$$\frac{\partial a(t)}{a(t)} = \frac{-i\lambda_j}{\hbar}dt \Bigg\} \quad \ln a(t) = -\frac{i\lambda_j}{\hbar}t \Rightarrow a(t) = e^{-\frac{i\lambda_j t}{\hbar}}$$

Solving Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

$|\psi(0)\rangle = |\phi_j\rangle$ where $|\phi_j\rangle$ is some eigenvector of H with a corresponding eigenvalue $|\lambda_j\rangle$

Then $|\psi(t)\rangle = e^{-\frac{i\lambda_j t}{\hbar}}|\phi_j\rangle$

$$|\psi(0)\rangle = \sum \alpha_j |\phi_j\rangle$$

$$|\psi(t)\rangle = \sum \alpha_j e^{-i\lambda_j t/\hbar} |\phi_j\rangle$$

$$|\psi(t)\rangle = \underbrace{\begin{pmatrix} e^{-i\lambda_0 t/\hbar} & & 0 \\ & \ddots & \\ 0 & & e^{-i\lambda_{k-1} t/\hbar} \end{pmatrix}}_{= \underline{\underline{U(t)}}} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{k-1} \end{pmatrix}$$

$$U(t) U(t)^{\dagger} = I.$$

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

$$B = e^{A}$$

A evectors $|\phi_i\rangle$ λ_i.

B evectors $|\phi_i\rangle$ e^{λ_i}

Solving Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

In general: $|\psi(0)\rangle = \sum_j \alpha_j|\phi_j\rangle$

$$|\psi(t)\rangle = \sum_j \alpha_j e^{-\frac{i\lambda_j t}{\hbar}}|\phi_j\rangle$$

In the eigenbasis, we can write

$$|\psi(t)\rangle = \underbrace{\begin{pmatrix} e^{-\frac{i\lambda_1 t}{\hbar}} & & 0 \\ & \ddots & \\ 0 & & e^{-\frac{i\lambda_k t}{\hbar}} \end{pmatrix}}_{= U(t)}|\psi(0)\rangle$$

unitary $U(t) = e^{-\frac{iHt}{\hbar}}$ (shorthand notation)

$UU^\dagger = U^\dagger U = I$

$B = e^A$

B has same evectors

evalue of A is λ_j

evalue of $B = e^{\lambda_j}$

Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

In general: $|\psi(0)\rangle = \sum \alpha_j |\phi_j\rangle$

$$|\psi(t)\rangle = \sum \alpha_j e^{-\frac{i\lambda_j t}{\hbar}} |\phi_j\rangle$$

Example $|\psi(0)\rangle = |0\rangle$

$H = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

What is $|\psi(t)\rangle$?

$|+\rangle \quad , \; 1$

$|-\rangle \quad , \; -1 .$

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

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-it/\hbar} |+\rangle + \frac{1}{\sqrt{2}} e^{it/\hbar} |-\rangle$$

$$t = \frac{\pi\hbar}{2}$$

$$\left|\psi\left(\frac{\pi\hbar}{2}\right)\right\rangle = \frac{1}{\sqrt{2}}(-i)|+\rangle + \frac{1}{\sqrt{2}}(i)|-\rangle$$

$$= -i\left[\frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}|-\rangle\right]$$

$$= \underline{\underline{-i|1\rangle}}$$