Operators, observables, and outcomes of measurements

Dirac's notation allows you to omit "$\cdot$ and $\otimes$"

$\langle\psi|\cdot|\varphi\rangle = (\alpha^* \; \beta^*)\cdot\begin{pmatrix}\gamma\\ \delta\end{pmatrix} = \alpha^*\gamma + \beta^*\delta$

OMIT

$\langle\psi|\cdot|\varphi\rangle \equiv \langle\psi|\varphi\rangle$

TO REMOVE AMBIGUITY

$\cancel{\langle\psi|\otimes|\varphi\rangle}$ NOT ALLOWED!

$|\psi\rangle\otimes|\varphi\rangle \equiv |\psi\rangle|\varphi\rangle$

$|\psi\rangle\otimes\langle\varphi| = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}\otimes(\gamma^* \; \delta^*) = \begin{pmatrix}\alpha(\gamma^* \; \delta^*)\\ \beta(\gamma^* \; \delta^*)\end{pmatrix} = \begin{pmatrix}\alpha\gamma^* & \alpha\delta^*\\ \beta\gamma^* & \beta\delta^*\end{pmatrix}$

$= |\psi\rangle\langle\varphi|$

Computational basis for qubits

- There exists an infinite set of possible choices for the basis (even for 1 qubit!). But one particular choice stands out for its simplicity, the *computational basis*. For 1 qubit it is given by $\{|0\rangle, |1\rangle\}$
- For 2 qubits: $\{\underbrace{|00\rangle}_{=0}, \underbrace{|01\rangle}_{=1}, \underbrace{|10\rangle}_{=2}, \underbrace{|11\rangle}_{=3}\}$ BASE 10

  $|0\rangle|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}1\\0\end{pmatrix}\\ 0\begin{pmatrix}1\\0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$

  $|1\rangle|0\rangle = \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ ← 3rd
- For n qubits the basis is the set of all $|j_1 j_2 j_3 \dots j_n\rangle$, with $j_i = 0$ or 1. There are 2^n elements in this basis (dimension $= \boxed{N=2^n}$) and they can be labelled by a single base 10 number $j = j_1 2^{n-1} + j_2 2^{n-2} + \cdots + j_n 2^0$:

$$\{|j\rangle\}_{j=0}^{2^n-1} = \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\} \text{ FOR 2 qubits!}$$

- The Hilbert space is exponentially large, and this (together with other properties) is what leads to "quantum advantage".

Changing the basis of a ket

$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

- Let's write this state in a new basis $\{|+\rangle, |-\rangle\}$:

$\begin{cases} |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{cases}$

COMPLETENESS: $|+\rangle\langle+| + |-\rangle\langle-| = I$ ← IDENTITY

$I|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

$|\psi\rangle = (|+\rangle\langle+| + |-\rangle\langle-|)[\alpha|0\rangle + \beta|1\rangle]$

$= \alpha(|+\rangle\underbrace{\langle+|0\rangle}_{=\frac{1}{\sqrt{2}}} + |-\rangle\underbrace{\langle-|0\rangle}_{=\frac{1}{\sqrt{2}}}) + \beta(|+\rangle\underbrace{\langle+|1\rangle}_{=\frac{1}{\sqrt{2}}} + |-\rangle\underbrace{\langle-|1\rangle}_{=-\frac{1}{\sqrt{2}}})$

$|\psi\rangle = \left(\frac{\alpha+\beta}{\sqrt{2}}\right)|+\rangle + \left(\frac{\alpha-\beta}{\sqrt{2}}\right)|-\rangle$

Matrices as Operators

- In quantum theory states = vectors. States can be manipulated by applying matrices on them, so *square matrices are called operators* (we put a hat on them to distinguish from c-numbers). For example the Pauli-X operator (also known as "quantum NOT"):

$$\hat{X} = |0\rangle\langle 1| + |1\rangle\langle 0| = \begin{pmatrix}1\\0\end{pmatrix}\otimes(0\;1) + \begin{pmatrix}0\\1\end{pmatrix}\otimes(1\;0) = \begin{pmatrix}0&1\\0&0\end{pmatrix} + \begin{pmatrix}0&0\\1&0\end{pmatrix} = \begin{pmatrix}0&1\\1&0\end{pmatrix}$$

- Using the computational basis $\{|j\rangle\}_{j=0}^{2^n-1}$ for n qubits:

$$\hat{A} = \sum_{i,j} A_{ij}|i\rangle\langle j|$$

$\hat{A} = \hat{I}\cdot\hat{A}\,\hat{I} = \left(\sum_i |i\rangle\langle i|\right)\hat{A}\left(\sum_j |j\rangle\langle j|\right)$

$= \sum_{ij} |i\rangle\underbrace{\langle i|\hat{A}|j\rangle}_{\equiv A_{ij}}\langle j|$

$\boxed{A_{ij} = \langle i|\hat{A}|j\rangle}$

$\boxed{\hat{A} = \sum_{ij}\langle i|\hat{A}|j\rangle\, |i\rangle\langle j|}$

Products of operators = usual product of matrices

$$\hat{A}\hat{B} = \hat{I}\hat{A}\hat{I}\hat{B}\hat{I} = \sum_{i,j,k}|i\rangle\langle i|\hat{A}|j\rangle\langle j|\hat{B}|k\rangle\langle k|$$

$$= \sum_{i,k}\left(\sum_j A_{ij}B_{jk}\right)|i\rangle\langle k|$$

- Note: Usually $\hat{A}\hat{B} \neq \hat{B}\hat{A}$! For example,

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

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

$\neq$!

Hermitian conjugate (or adjoint) of Â: Â† ← "Dagger" $A^\dagger$

- The "$\dagger$" of an operator is the conjugate + transpose of its matrix:

$\hat{A} = \begin{pmatrix}\alpha&\beta\\ \gamma&\delta\end{pmatrix}$ $\hat{A}^\dagger = \begin{pmatrix}\alpha^*&\gamma^*\\ \beta^*&\delta^*\end{pmatrix}$

$(|+\rangle)^\dagger = \langle+|$ $(\langle+|)^\dagger = |+\rangle$

$\boxed{\left(\hat{A}|\Psi\rangle\right)^\dagger = \langle\Psi|\hat{A}^\dagger}$

$(\langle\psi|\varphi\rangle)^\dagger = \langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^*$

- Hermitian operators are the ones that satisfy

$$\boxed{\hat{A} = \hat{A}^\dagger}$$

$\hat{A} = \sum_{ij}\langle i|\hat{A}|j\rangle\, |i\rangle\langle j| \xrightarrow{\dagger} \hat{A}^\dagger = \sum_{ij}\langle i|\hat{A}|j\rangle^*\, |j\rangle\langle i| = \sum_{ij}\langle j|\hat{A}|i\rangle^* |i\rangle\langle j|$ $i \rightleftarrows j$

$\hat{A}^\dagger = \sum_{ij}\underbrace{\langle i|\hat{A}^\dagger|j\rangle}_{=\langle j|\hat{A}|i\rangle^*}|i\rangle\langle j|$

$\boxed{(A^\dagger)_{ij} = (A)^*_{ji}}$

Diagonalization with a change of basis

- Consider the Pauli-X operator again: $\hat{X} = |0\rangle\langle 1| + |1\rangle\langle 0|$
- Let's write it in a new basis $\{|+\rangle, |-\rangle\}$:

$\begin{cases} |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{cases}$

$|S_x,+\rangle = |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$

$|S_x,-\rangle = -|-\rangle$

REPRESENT USING $\{|+\rangle, |-\rangle\}$ AS BASIS: $\begin{pmatrix}1\\0\end{pmatrix}$ $\begin{pmatrix}0\\1\end{pmatrix}$

$\hat{X} = (|+\rangle\langle+| + |-\rangle\langle-|)\,\hat{X}\,(|+\rangle\langle+| + |-\rangle\langle-|)$

$= |+\rangle\underbrace{\langle+|\hat{X}|+\rangle}_{=1}\langle+| + |+\rangle\underbrace{\langle+|\hat{X}|-\rangle}_{=0}\langle-| + |-\rangle\underbrace{\langle-|\hat{X}|+\rangle}_{=0}\langle+| + |-\rangle\underbrace{\langle-|\hat{X}|-\rangle}_{=-1}\langle-|$

$= \sum_{a=+1,-1} a|a\rangle\langle a| = |+\rangle\langle+| - |-\rangle\langle-|$ $\hat{X} = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$ IN $|\pm\rangle$ BASIS

- Note how $\{|+\rangle, |-\rangle\}$ are eigenvectors of $\hat{X}$:

$\hat{X}|+\rangle = (+1)|+\rangle$

$\hat{X}|-\rangle = (-1)|-\rangle = -|-\rangle$

Which operators are diagonalizable?

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

- We can prove that an operator can be diagonalized if and only if it satisfies the *normal property*:

$$\boxed{\hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A}}$$

- The proof is advanced (p. 72 Nielsen & Chuang). Important corollary: If Â is Hermitian, it can be diagonalized and all it eigenvalues are real!

$\hat{A} = \hat{A}^\dagger \Rightarrow \hat{A}$ IS NORMAL!

$\langle i|\hat{A}|j\rangle = \langle j|\hat{A}|i\rangle^* \Rightarrow$ DIAGONALS $(i=j)$ ARE REAL!

$\hat{A} = \hat{A}^\dagger \Rightarrow A_{ij} = A^*_{ji} \Rightarrow A_{ii} = A^*_{ii}$ A_{ii} is real!

IF $\hat{A} = \hat{A}^\dagger \Rightarrow \hat{A}$ IS DIAGONALIZABLE AND ALL EIGENVALUES ARE REAL!

Measurements, observables, and Hermitian operators

- An important postulate of quantum theory is that the outcome of a measurement is always one of the eigenvalues of the observable we are measuring. Since anything we measure in the lab - e.g. spin in S-G exp. or current in a superconducting circuit – is a real number, *all observables must be Hermitian operators*. For example, the spin operator:

$$\hat{S} = \frac{\hbar}{2}(\hat{X}, \hat{Y}, \hat{Z})$$

$\hbar = \frac{h}{2\pi}$ → PLANCK'S CONSTANT

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

$\hat{Y} = \begin{pmatrix}0&-i\\i&0\end{pmatrix}$ PAULI-Y

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

Summary

- States = vectors (kets)
- Operators = square matrices (Â, Ô, etc). They take one state into another:

$$\hat{A}|\Psi\rangle = |\Phi\rangle$$

- Operators can be represented by a matrix that depends on the basis of your choice. "Diagonalizable" operators are represented by a diagonal matrix when the basis = set of their eigenvectors.
- Hermitian operators satisfy

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

- Only normal operators are diagonalizable. They satisfy

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

- Hermitian $\Rightarrow$ normal. Therefore, Hermitian operators always have real eigenvalues. They represent physical quantities that we can measure (observables).