QUANTUM MECHANICS FOUNDATIONS OF QUANTUM INFORMATION PROCESSING

OPERATORS

SECOND POSTULATE

Every measurable physical quantity $\mathscr{A}$ is described by an operator $\hat{A}$ acting on $\mathcal{H}$; this operator is an observable.

An operator $\hat{A} : \mathcal{H} \to \mathcal{F}$ such that $|\psi'\rangle = \hat{A}|\psi\rangle$ for

$$|\psi\rangle \in \underbrace{\mathcal{H}}_{\text{domain } D(\hat{A})}$$

and $$|\psi'\rangle \in \underbrace{\mathcal{F}}_{\text{range } R(\hat{A})}$$

Properties:

1. Linearity $\hat{A} \sum_i c_i|\phi_i\rangle = \sum_i c_i\hat{A}|\phi_i\rangle$

2. Equality $\hat{A} = \hat{B}$ iff $\hat{A}|\psi\rangle = \hat{B}|\psi\rangle$ and $D(\hat{A}) = D(\hat{B})$

3. Sum $\hat{C} = \hat{A} + \hat{B}$ iff $\hat{C}|\psi\rangle = \hat{A}|\psi\rangle + \hat{B}|\psi\rangle$

4. Product $\hat{C} = \hat{A}\hat{B}$ iff

$$\begin{aligned} \hat{C}|\psi\rangle &= \hat{A}\hat{B}|\psi\rangle \\ &= \hat{A}\left(\hat{B}|\psi\rangle\right) = \hat{A}|\hat{B}\psi\rangle \end{aligned}$$

5. <u>Functions</u> $\hat{A}^2 = \hat{A}\hat{A}$, then $\hat{A}^n = \hat{A}\hat{A}^{n-1}$ and if a function $f(\xi) = \sum_n a_n \xi^n$, then by the function of an operator $f(\hat{A})$ we mean

$$f\left(\hat{A}\right) = \sum_n a_n \hat{A}^n$$

e.g.

$$e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{1}{n!} \hat{A}^n$$

We will see later how to calculate a function of an operator using its spectral decomposition.

Iff the operator is diagonal, the function of the operator is obtained by taking the function of each of its diagonal elements, its eigenvalues.

Example:

Let

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

then

$$\hat{S} = \sqrt{\hat{Z}} = \begin{pmatrix} \sqrt{1} & 0 \\ 0 & \sqrt{-1} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix}$$

Commutator and anticommutator

In contrast to numbers, a product of operators is generally not commutative, i.e.

$$\hat{A}\hat{B} \quad \neq \quad \hat{B}\hat{A}$$

For example: three vectors $|x\rangle$, $|y\rangle$ and $|z\rangle$ and two operators $\hat{R}_x$ and $\hat{R}_y$ such that:

$$\begin{array}{ll} \hat{R}_x|x\rangle = |x\rangle, & \hat{R}_y|x\rangle = -|z\rangle, \\ \hat{R}_x|y\rangle = |z\rangle, & \hat{R}_y|y\rangle = |y\rangle, \\ \hat{R}_x|z\rangle = -|y\rangle, & \hat{R}_y|z\rangle = |x\rangle \end{array}$$

then

$$\hat{R}_x\hat{R}_y|z\rangle = \hat{R}_x|x\rangle = |x\rangle \quad \neq$$

$$\hat{R}_y\hat{R}_x|z\rangle = -\hat{R}_y|y\rangle = -|y\rangle$$

An operator $\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$ is called <u>commutator</u>.
We say that $\hat{A}$ and $\hat{B}$ commute iff $\left[\hat{A},\hat{B}\right]=0$ in which case also $\left[f(\hat{A}),f(\hat{B})\right]=0$.
An operator $\left\{\hat{A},\hat{B}\right\}=\hat{A}\hat{B}+\hat{B}\hat{A}$ is called <u>anticommutator</u>.

Basic properties:

$$\begin{aligned}\left[\hat{A},\hat{B}\right] &= -\left[\hat{B},\hat{A}\right]\\ \left\{\hat{A},\hat{B}\right\} &= \left\{\hat{B},\hat{A}\right\}\\ \left[\hat{A},\hat{B}+\hat{C}\right] &= \left[\hat{A},\hat{B}\right]+\left[\hat{A},\hat{C}\right]\\ \left[\hat{A},\hat{B}\hat{C}\right] &= \left[\hat{A},\hat{B}\right]\hat{C}+\hat{B}\left[\hat{A},\hat{C}\right]\end{aligned}$$

the Jacobi identity:

$$\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right] = 0$$

Types of operators (examples)

1. $\hat{A}$ is bounded iff $\exists \beta > 0$ such that $\left\| \hat{A}|\psi\rangle \right\| \leq \beta \, \| |\psi\rangle \|$ for all $|\psi\rangle \in D(\hat{A})$. Infimum of β is called the norm of $\hat{A}$

2. $\hat{A}$ is symmetric if $\langle \psi_1 | \hat{A} \psi_2 \rangle = \langle \hat{A} \psi_1 | \psi_2 \rangle$ for all $|\psi_1\rangle, |\psi_2\rangle \in D(\hat{A})$.

3. $\hat{A}$ is hermitian if it is bounded and symmetric.

4. Let $\hat{A}$ be a bounded operator (with $D(\hat{A})$ dense in $\mathcal{H}$); then there is an adjoint operator $\hat{A}^\dagger$ such that

$$\langle \psi_1 | \hat{A}^\dagger \psi_2 \rangle \quad = \quad \langle \hat{A} \psi_1 | \psi_2 \rangle$$

i.e.

$$\langle \psi_1 | \hat{A}^\dagger \psi_2 \rangle = \langle \psi_2 | \hat{A} \psi_1 \rangle^*$$

for all $|\psi_1\rangle, |\psi_2\rangle \in D(\hat{A})$.

Properties:

$$\begin{aligned}
\left\| \hat{A}^\dagger \right\| &= \|\hat{A}\| \\
\left(\hat{A}^\dagger\right)^\dagger &= \hat{A} \\
\left(\hat{A} + \hat{B}\right)^\dagger &= \hat{A}^\dagger + \hat{B}^\dagger \\
\left(\hat{A}\hat{B}\right)^\dagger &= \hat{B}^\dagger \hat{A}^\dagger \text{ (the order changes)} \\
\left(\lambda \hat{A}\right)^\dagger &= \lambda^* \hat{A}^\dagger
\end{aligned}$$

How can we construct an adjoint?
E.g. Let us have an operator in a matrix representation (so it is also a matrix) then

$$\hat{A}^\dagger = \left(A^{\mathrm{T}}\right)^* \quad = \quad \text{transpose \& complex conjugation}$$

5. $\hat{A}$ is selfadjoint if $\hat{A}^\dagger = \hat{A}$.
   This is the property of observables!
   Their eigenvalues are real numbers, e.g. $\hat{X}|x\rangle = x|x\rangle$

6. $\hat{A}$ is positive if $\langle\psi|\hat{A}|\psi\rangle \geq 0$ for all $|\psi\rangle \in \mathcal{H}$

7. $\hat{A}$ is normal if $\hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A}$ i.e. $\underbrace{\left[\hat{A}, \hat{A}^\dagger\right] = 0}_{\text{commutator}}$

8. Let $\hat{A}$ be an operator. If there exists an operator $\hat{A}^{-1}$ such that $\hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = \hat{1}$ (identity operator) then $\hat{A}^{-1}$ is called an inverse operator to $\hat{A}$

   Properties:

$$
\begin{aligned}
\left(\hat{A}\hat{B}\right)^{-1} &= \hat{B}^{-1}\hat{A}^{-1} \\
\left(\hat{A}^{\dagger}\right)^{-1} &= \left(\hat{A}^{-1}\right)^{\dagger}
\end{aligned}
$$

9. an operator $\hat{U}$ is called unitary if $\hat{U}^{\dagger} = \hat{U}^{-1}$, i.e. $\hat{U}\hat{U}^{\dagger} = \hat{U}^{\dagger}\hat{U} = \hat{1}$.

   Formal solution of the Schrödinger equation leads to a unitary operator: if $\hat{H}$ is the Hamiltonian (total energy operator),

$$
\begin{aligned}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle &= \hat{H}|\psi(t)\rangle \\
\Rightarrow \int_0^t \frac{\mathrm{d}|\psi(t')\rangle}{|\psi(t')\rangle} &= -\frac{i}{\hbar}\int_0^t \hat{H}\mathrm{d}t'
\end{aligned}
$$

If the Hamiltonian is time independent then

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle = \hat{U}|\psi(0)\rangle$$

10. An operator $\hat{P}$ satisfying $\hat{P} = \hat{P}^{\dagger} = \hat{P}^2$ is a <u>projection operator</u> or <u>projector</u> e.g. if $|\psi_k\rangle$ is a normalized vector then

$$\hat{P}_k = |\psi_k\rangle\langle\psi_k|$$

is the projector onto one-dimensional space spanned by all vectors linearly dependent on $|\psi_k\rangle$.

Matrix representation of quantum computing operations

Matrix representation in general

Operator is uniquely defined by its action on the basis vectors of the Hilbert space.
Let $\mathcal{B} = \left\{|\psi_j\rangle\right\}$ be a basis of $\mathcal{H}$ $(= D(\hat{A}))$

$$\begin{aligned}\hat{A}|\psi_j\rangle &= \sum_k |\psi_k\rangle\langle\psi_k|\hat{A}|\psi_j\rangle \\ &= \sum_k A_{kj}|\psi_k\rangle\end{aligned}$$

where $A_{kj} = \langle\psi_k|\hat{A}|\psi_j\rangle$ are the matrix elements of the operator $\hat{A}$ in the matrix representation given by the basis $\mathcal{B}$.
For practical calculations

$$\hat{A} = \sum_{kj} |\psi_k\rangle\langle\psi_k|\hat{A}|\psi_j\rangle\langle\psi_j| = \sum_{kj} A_{kj}|\psi_k\rangle\langle\psi_j|$$

Single-qubt operations in the standard computational basis

(i) Phase flip

$$\begin{aligned}
\hat{Z} &= \left(\sum_{k=0,1} |k\rangle\langle k|\right)\hat{Z}\left(\sum_{l=0,1} |l\rangle\langle l|\right) = \sum_{k,l}\langle k|\hat{Z}|l\rangle\ |k\rangle\langle l| \\
&= \langle 0|\hat{Z}|0\rangle|0\rangle\langle 0| + \langle 0|\hat{Z}|1\rangle|0\rangle\langle 1| + \langle 1|\hat{Z}|0\rangle|1\rangle\langle 0| + \langle 1|\hat{Z}|1\rangle|1\rangle\langle 1| \\
&= \langle 0|\hat{Z}|0\rangle\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + \langle 0|\hat{Z}|1\rangle\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} \\
&+ \langle 1|\hat{Z}|0\rangle\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + \langle 1|\hat{Z}|1\rangle\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} \langle 0|\hat{Z}|0\rangle & \langle 0|\hat{Z}|1\rangle \\ \langle 1|\hat{Z}|0\rangle & \langle 1|\hat{Z}|1\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z
\end{aligned}$$

(ii) Bit flip

$$\hat{X} = \begin{pmatrix} \langle 0|\hat{X}|0\rangle & \langle 0|\hat{X}|1\rangle \\ \langle 1|\hat{X}|0\rangle & \langle 1|\hat{X}|1\rangle \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x$$

(iii) $\hat{Y} = i\hat{Z}\hat{X}$

$$\hat{Y} = \begin{pmatrix} \langle 0|\hat{Y}|0\rangle & \langle 0|\hat{Y}|1\rangle \\ \langle 1|\hat{Y}|0\rangle & \langle 1|\hat{Y}|1\rangle \end{pmatrix} = \begin{pmatrix} \langle 0|i\hat{Z}\hat{X}|0\rangle & \langle 0|i\hat{Z}\hat{X}|1\rangle \\ \langle 1|i\hat{Z}\hat{X}|0\rangle & \langle 1|i\hat{Z}\hat{X}|1\rangle \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y$$

(iv) $\hat{S} = \sqrt{\hat{Z}}$

$$\hat{S} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

(v) $\hat{T} = \sqrt{\hat{S}}$

$$\hat{T} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

(vi) Hadamard gate

$$\hat{H} = \begin{pmatrix} \langle 0|\hat{H}|0\rangle & \langle 0|\hat{H}|1\rangle \\ \langle 1|\hat{H}|0\rangle & \langle 1|\hat{H}|1\rangle \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)$$

Two-qubt operations in the standard computational basis

(i) $CNOT_{12}$ (the first qubit is the control qubit, the second is the target):

$$CNOT_{12} \quad = \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = |0\rangle\langle 0| \otimes \hat{I} + |1\rangle\langle 1| \otimes \hat{X} = \hat{P}_0 \otimes \hat{I} + \hat{P}_1 \otimes \hat{X}$$

(ii) $CNOT_{21}$:

$$CNOT_{21} \quad = \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} = \hat{I} \otimes |0\rangle\langle 0| + \hat{X} \otimes |1\rangle\langle 1| = \hat{I} \otimes \hat{P}_0 + \hat{X} \otimes \hat{P}_1$$

(iii) $SWAP = CNOT_{12}CNOT_{21}CNOT_{12}$

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

Composition of operators (by example)

1. Direct sum $\hat{A} = \hat{B} \oplus \hat{C}$

   $\hat{B}$ acts on $\mathcal{H}_B$ (2 dimensional) and $\hat{C}$ acts on $\mathcal{H}_C$ (3 dimensional)

   Let

$$\hat{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \quad \text{and} \quad \hat{C} = \begin{pmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{pmatrix}$$

$$\hat{A} \quad = \begin{pmatrix} b_{11} & b_{12} & 0 & 0 & 0 \\ b_{21} & b_{22} & 0 & 0 & 0 \\ 0 & 0 & c_{11} & c_{12} & c_{13} \\ 0 & 0 & c_{21} & c_{22} & c_{23} \\ 0 & 0 & c_{31} & c_{32} & c_{33} \end{pmatrix}$$

   Acts on $\mathcal{H}_B \oplus \mathcal{H}_C$

Properties:

$$\begin{aligned} \mathrm{Tr}\left(\hat{B} \oplus \hat{C}\right) &= \mathrm{Tr}\left(\hat{B}\right) + \mathrm{Tr}\left(\hat{C}\right) \\ \det\left(\hat{B} \oplus \hat{C}\right) &= \det\left(\hat{B}\right) \det\left(\hat{C}\right) \end{aligned}$$

2. Direct product $\hat{A} = \hat{B} \otimes \hat{C}$:

$$|\psi\rangle \in \mathcal{H}_B,\ |\phi\rangle \in \mathcal{H}_C, \qquad |\chi\rangle \in \mathcal{H}_B \otimes \mathcal{H}_C$$

$$\begin{aligned} \hat{A}|\chi\rangle &= \left(\hat{B} \otimes \hat{C}\right) \underbrace{(|\psi\rangle \otimes |\phi\rangle)}_{|\psi\rangle|\phi\rangle \text{ to simplify the notation}} \\ &= \hat{B}|\psi\rangle \hat{C}|\phi\rangle \end{aligned}$$

$$\hat{A} = \begin{pmatrix} b_{11}c_{11} & b_{11}c_{12} & b_{11}c_{13} & b_{12}c_{11} & b_{12}c_{12} & b_{12}c_{13} \\ b_{11}c_{21} & b_{11}c_{22} & b_{11}c_{23} & b_{12}c_{21} & b_{12}c_{22} & b_{12}c_{23} \\ b_{11}c_{31} & b_{11}c_{32} & b_{11}c_{33} & b_{12}c_{31} & b_{12}c_{32} & b_{12}c_{33} \\ b_{21}c_{11} & b_{21}c_{12} & b_{21}c_{13} & b_{22}c_{11} & b_{22}c_{12} & b_{22}c_{13} \\ b_{21}c_{21} & b_{21}c_{22} & b_{21}c_{23} & b_{22}c_{21} & b_{22}c_{22} & b_{22}c_{23} \\ b_{21}c_{31} & b_{21}c_{32} & b_{21}c_{33} & b_{22}c_{31} & b_{22}c_{32} & b_{22}c_{33} \end{pmatrix}$$

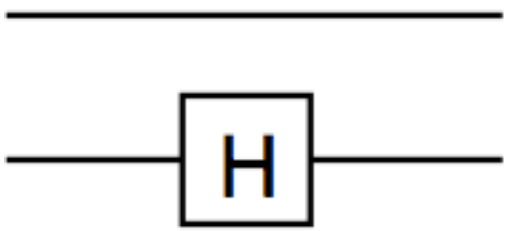
Examples Hadamard gates

$$\hat{H} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

on two qubit states:

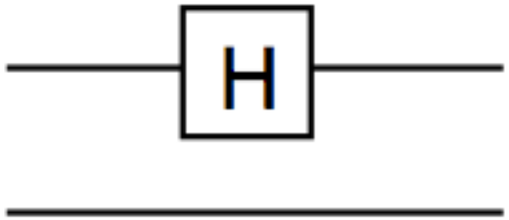
(i) Hadamard gate on the second qubit:

$$\hat{I} \otimes \hat{H} = \begin{pmatrix} 1.\hat{H} & 0.\hat{H} \\ 0.\hat{H} & 1.\hat{H} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$



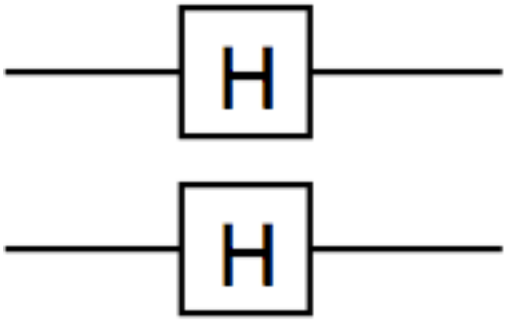
(ii) Hadamard gate on the first qubit:

$$\hat{H} \otimes \hat{I} = \begin{pmatrix} \frac{1}{\sqrt{2}}.\hat{I} & \frac{1}{\sqrt{2}}.\hat{I} \\ \frac{1}{\sqrt{2}}.\hat{I} & -\frac{1}{\sqrt{2}}.\hat{I} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}$$



(iii) Hadamard gates on both qubits:

$$\hat{H} \otimes \hat{H} = \begin{pmatrix} \frac{1}{\sqrt{2}}.\hat{H} & \frac{1}{\sqrt{2}}.\hat{H} \\ \frac{1}{\sqrt{2}}.\hat{H} & -\frac{1}{\sqrt{2}}.\hat{H} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$



Eigenvalues and eigenvectors

Solving a quantum mechanical system means to find the eigenvalues and eigenvectors of the complete set of commuting observables (C.S.C.O.)

1. The eigenvalue equation

$$\hat{A}|\psi_\alpha\rangle = \underbrace{\alpha}_{\text{eigenvalue}} \underbrace{|\psi_\alpha\rangle}_{\text{eigenvector}}$$

   If $n > 1$ vectors satisfy the eigenvalue equation for the same eigenvalue α, we say the eigenvalue is n-fold degenerate.

2. The eigenvalues of a self-adjoint operator $\hat{A}$, which are observables and represent physical quantities, are real numbers

$$\begin{aligned}
\alpha\langle\psi_\alpha|\psi_\alpha\rangle &= \langle\psi_\alpha|\hat{A}\psi_\alpha\rangle \\
&= \langle\hat{A}\psi_\alpha|\psi_\alpha\rangle^* = \alpha^*\langle\psi_\alpha|\psi_\alpha\rangle \\
\Rightarrow \alpha = \alpha^* &\Rightarrow \alpha \in \mathbb{R}
\end{aligned}$$

3. Eigenvectors of self-adjoint operators corresponding to distinct eigenvalues are orthogonal.
   Proof: if $\beta \neq \alpha$ is also an eigenvalue of $\hat{A}$ then

$$\langle \psi_\alpha | \hat{A} \psi_\beta \rangle = \beta \langle \psi_\alpha | \psi_\beta \rangle$$

   and also

$$\begin{aligned} \langle \psi_\alpha | \hat{A} \psi_\beta \rangle &= \langle \psi_\beta | \hat{A} \psi_\alpha \rangle^* \\ &= \alpha^* \langle \psi_\beta | \psi_\alpha \rangle^* = \alpha \langle \psi_\alpha | \psi_\beta \rangle \end{aligned}$$

   which implies

$$\langle \psi_\alpha | \psi_\beta \rangle = 0$$

Spectral decomposition of an operator

Assume that the eigenvectors of $\hat{A}$ define a basis $\mathcal{B} = \left\{|\psi_j\rangle\right\}$,
then $A_{kj} = \langle\psi_k|\hat{A}|\psi_j\rangle = \alpha_j\delta_{kj}$.
Operator in this basis is a diagonal matrix with eigenvalues on the diagonal

$$
\begin{aligned}
\hat{A} &= \sum_{kj} A_{kj}|\psi_k\rangle\langle\psi_j| \\
&= \sum_{j} \alpha_j|\psi_j\rangle\langle\psi_j| \\
&= \sum_{j} \alpha_j\hat{E}_j
\end{aligned}
$$

$\hat{E}_j$ is a projector onto 1-dim. space spanned by $|\psi_j\rangle \Rightarrow$ Spectral decomposition!

Function of an operator using its spectral decomposition

$$f(\hat{A}) \;=\; \sum_j f(\alpha_j)|\psi_j\rangle\langle\psi_j| = \sum_j f(\alpha_j)\hat{E}_j$$

If and only if the operator is diagonal, the function of the operator is obtained by taking the function of each of its diagonal elements, its eigenvalues.

<u>Example:</u>

$$\hat{S} \;=\; \sqrt{\hat{Z}} = \begin{pmatrix} \sqrt{1} & 0 \\ 0 & \sqrt{-1} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix}$$