Standard computational basis

1 qubit: the dimension of the Hilbert space: $d = 2^1$

The standard computational basis

$$\mathcal{B} = \{|0\rangle, |1\rangle\}$$

- orthogonality:

$$\langle 0|1\rangle \quad = \quad \langle 1|0\rangle = 0$$

- normalization:

$$\langle 0|0\rangle \quad = \quad \langle 1|1\rangle = 1$$

- or both using the Kronecker delta:

$$\langle i|j\rangle \quad = \quad \delta_{ij}$$

2 qubits: the dimension of the Hilbert space: $d = 2^2$
The standard computational basis

$$\mathcal{B} = \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$$

- orthogonality:

$$\begin{aligned} \langle 00|01\rangle &= \langle 01|00\rangle = 0 \quad \langle 00|10\rangle = \langle 10|00\rangle = 0 \quad \langle 00|11\rangle = \langle 11|00\rangle = 0 \\ \langle 01|10\rangle &= \langle 10|01\rangle = 0 \quad \langle 01|11\rangle = \langle 11|01\rangle = 0 \quad \langle 10|11\rangle = \langle 11|10\rangle = 0 \end{aligned}$$

-normalization:

$$\langle 00|00\rangle = \langle 01|01\rangle = \langle 10|10\rangle = \langle 11|11\rangle = 1$$

or using the Kronecker delta

$$\langle i_1 i_2 | j_1 j_2 \rangle = \delta_{i_1 j_1} \delta_{i_2 j_2}$$

n qubits: the dimension of the Hilbert space: $d = 2^n$

The standard computational basis

$$\mathcal{B} = \{|0\ldots00\rangle, |0\ldots01\rangle, \ldots, |1\ldots10\rangle, |1\ldots11\rangle\}$$

- orthonormality

$$\langle i_1 i_2 \ldots i_n | j_1 j_2 \ldots i_n \rangle = \delta_{i_1 j_1} \delta_{i_2 j_2} \ldots \delta_{i_n j_n}$$

Example: the standard basis of a three-qubit Hilbert space

$$\mathcal{B} = \{|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle\}$$

Standard basis in matrix representation

Example: 1 qubit

$$\mathcal{B} = \{|0\rangle, |1\rangle\}$$

$$\mathcal{B} = \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$$

Example: 2 qubits

$$\mathcal{B} = \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$$

$$\mathcal{B} = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

Example: 3 qubits

$$\mathcal{B} = \{|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle\}$$

$$\mathcal{B} = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

Representation of a quantum mechanical state

We will first introduce the **completeness relation** which is a useful way of expressing an identity operator on the Hilbert space.

Consider the standard computational basis as an example, the completeness relation has the form

$$|0\rangle\langle 0| + |1\rangle\langle 1| = \hat{1}$$

We use it to define the representations of $|\psi\rangle$

$$\begin{aligned}
|\psi\rangle &= \hat{1}\,|\psi\rangle = (|0\rangle\langle 0| + |1\rangle\langle 1|)\,|\psi\rangle \\
&= |0\rangle\langle 0|\psi\rangle + |1\rangle\langle 1|\psi\rangle \\
&= \langle 0|\psi\rangle\,|0\rangle + \langle 1|\psi\rangle\,|1\rangle \\
&= c_0|0\rangle + c_1|1\rangle
\end{aligned}$$

where the probability amplitudes are explicitly $c_0 = \langle 0|\psi\rangle$ and $c_1 = \langle 1|\psi\rangle$.

It is easy to verify in our case that the completeness relation is an identity operator using the matrix representation

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

More generally, the **completeness relation** is given as

$$\sum_i |\phi_i\rangle\langle\phi_i| = \hat{1}$$

where the sum goes over all basis vectors $\mathcal{B} = \{|\phi_1\rangle, |\phi_2\rangle \ldots\}$.

Our state can now be expanded into a a specific superposition of the basis vectors $\{|\phi_i\rangle\}$

$$|\psi\rangle = \sum_i |\phi_i\rangle \underbrace{\langle\phi_i|\psi\rangle}_{\text{a number } c_i \in \mathbb{C}} = \sum_i c_i\, |\phi_i\rangle$$

Operators

An adjoint operator $\hat{A}^\dagger$ of a bounded operator $\hat{A}$ is such that $\langle\psi_1|\hat{A}\psi_2\rangle = \langle\hat{A}^\dagger\psi_1|\psi_2\rangle$ for all $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$. Properties:

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

In finite dimensions, an operator can be represented as a matrix and its adjoint is then obtained by

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

Examples of types of operators

1. An operator $\hat{A}$ is called **hermitian** or **selfadjoint** if $\hat{A}^\dagger = \hat{A}$, or $\langle \hat{A}\phi|\psi\rangle = \langle \phi|\hat{A}\psi\rangle$.

This is the property of quantum observables which can represent physical quantities. Their eigenvalues are real numbers, for example the Hamiltonian representing total energy of a quantum mechanical system and has the following eigenvalue equation

$$\hat{H}|E\rangle = E|E\rangle$$

where E are the eigenvalues and $|E\rangle$ are the corresponding eigenvectors.

2. 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:

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

3. An operator $\hat{U}$ is called **unitary** if $\hat{U}^{\dagger} = \hat{U}^{-1}$, that is $\hat{U}\hat{U}^{\dagger} = \hat{U}^{\dagger}\hat{U} = \hat{1}$.

Example: Quantum evolution operator

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

4. An operator $\hat{P}$ satisfying $\hat{P} = \hat{P}^{\dagger} = \hat{P}^{2}$ is a **projection operator** or **projector**
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 $|\psi_k\rangle$.

Example:

$$\hat{P}_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad \hat{P}_1 = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Matrix representation

Operator is uniquely defined by its action on the basis vectors of the Hilbert space.

Let $\mathcal{B} = \left\{|\phi_j\rangle\right\}$ be a basis of a finite-dimensional $\mathcal{H}$. Consider the completeness relation

$$\sum_i |\phi_i\rangle\langle\phi_i| = \hat{1}$$

and apply it as an identity onto an operator $\hat{A}$ from both sides

$$\hat{A} = \sum_{kj} |\phi_k\rangle\langle\phi_k|\hat{A}|\phi_j\rangle\langle\phi_j| = \sum_{kj} A_{kj}|\phi_k\rangle\langle\phi_j|$$

where $A_{kj} = \langle\phi_k|\hat{A}|\phi_j\rangle$ are the matrix elements of the operator $\hat{A}$ in the matrix representation given by the basis $\mathcal{B}$, and the operators $|\phi_k\rangle\langle\phi_j|$ correspond to the position of the corresponding matrix element in the matrix in this representation.

Example: the bit flip gate

$$X|0\rangle = |1\rangle \qquad X|1\rangle = |0\rangle.$$

The matrix representation

$$\begin{aligned}
X &= (|0\rangle\langle 0| + |1\rangle\langle 1|)X(|0\rangle\langle 0| + |1\rangle\langle 1|) \\
&= |0\rangle\langle 0|X|0\rangle\langle 0| + |0\rangle\langle 0|X|1\rangle\langle 1| + |1\rangle\langle 1|X|0\rangle\langle 0| + |1\rangle\langle 1|X|1\rangle\langle 1| \\
&= \langle 0|X|0\rangle|0\rangle\langle 0| + \langle 0|X|1\rangle|0\rangle\langle 1| + \langle 1|X|0\rangle|1\rangle\langle 0| + \langle 1|X|1\rangle|1\rangle\langle 1| \\
&= \langle 0|1\rangle|0\rangle\langle 0| + \langle 0|0\rangle|0\rangle\langle 1| + \langle 1|1\rangle|1\rangle\langle 0| + \langle 1|0\rangle|1\rangle\langle 1| \\
&= 0 \cdot |0\rangle\langle 0| + 1 \cdot |0\rangle\langle 1| + 1 \cdot |1\rangle\langle 0| + 0 \cdot |1\rangle\langle 1| \\
&= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}
\end{aligned}$$

Eigenvalues and eigenvectors

Finding the eigenvalues and eigenvectors of operators is essential in quantum mechanics.

We say that an operator $\hat{A}$ satisfies the eigenvalue equation if the following holds

$$\hat{A}|\psi_j\rangle = \underbrace{\alpha_j}_{\text{eigenvalue}} \underbrace{|\psi_j\rangle}_{\text{eigenvector}}$$

where $|\psi_j\rangle$ is the eigenvector that corresponds to the eigenvalue α_j. Since the eigenvalues are numbers, the eigenvalue equation means that a result of the action of an operator onto its eigenvector is proportional to the eigenvector.

Spectral decomposition of an operator

Every operator can be diagonalised, that is expressed in terms of the eigenvalues and eigenvectors in the following form: assume that the basis in the Hilbert space is chosen to be defined in terms of the eigenvectors of $\hat{A}$, that is in terms of the basis satisfying $\hat{A}|\psi_j\rangle = \alpha_j|\psi_j\rangle$, then the operator can be written as

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

This is the spectral decomposition.

Spectral decomposition of an operator $\hat{A}$

$$\hat{A} = \sum_j \alpha_j |\psi_j\rangle\langle\psi_j|$$

corresponds to a diagonal matrix because the operators $|\psi_j\rangle\langle\psi_j|$ correspond to diagonal elements in the matrix

$$\hat{A} = \sum_j \alpha_j |\psi_j\rangle\langle\psi_j| = \begin{pmatrix} \alpha_1 & 0 & 0 & \dots \\ 0 & \alpha_2 & 0 & \dots \\ 0 & 0 & \alpha_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Example: Phase-flip gate Z in the standard computational basis $\mathcal{B} = \{|0\rangle, |1\rangle\}$:

$$Z = (+1)|0\rangle\langle 0| + (-1)|1\rangle\langle 1| = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$$

Functions of operators

It is particularly easy to calculate functions of operators if they are given by their spectral decomposition:

$$f\left(\hat{A}\right) = \sum_j f(\alpha_j)|\psi_j\rangle\langle\psi_j| = \begin{pmatrix} f(\alpha_1) & 0 & 0 & \dots \\ 0 & f(\alpha_2) & 0 & \dots \\ 0 & 0 & f(\alpha_3) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

To calculate a function of an operator if it is not given in a diagonal form requires first to diagonalise the operator, then calculate the function and at the end transform it back to the original representation.