

Quantum Computation (CO484)

Quantum States and Evolution

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Quantum Postulates

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- ▶ The only **possible** results are eigen-values λ_i of \mathbf{A} .
- ▶ The **probability** of measuring λ_n in state $|x\rangle$ is given by:

$$Pr(A = \lambda_n | x) = \langle x | \mathbf{P}_n | x \rangle = \langle x | | \mathbf{P}_n x \rangle$$

with $\mathbf{P}_n = |\lambda_n\rangle\langle\lambda_n|$ the orthogonal projection onto the space generated by eigen-vector $|\lambda_n\rangle = |n\rangle$ of \mathbf{A} .

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A **complex number** $z \in \mathbb{C}$ is a (formal) combinations of two reals $x, y \in \mathbb{R}$:

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with $i^2 = -1$ or $i = \sqrt{-1}$. The **complex conjugate** of a complex number $z = x + iy \in \mathbb{C}$ is:

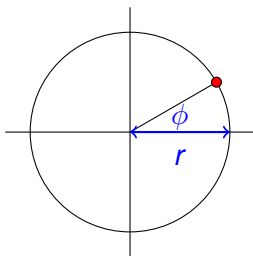
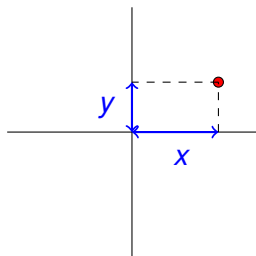
$$z^* = \bar{z} = \overline{x + iy} = x - iy = z^\dagger$$

Hauptsatz of Algebra

Complex numbers are algebraically closed: Every polynomial of order n over \mathbb{C} has exactly n roots.

Polar Coordinates

One can represent numbers $z \in \mathbb{C}$ using the complex plane.



Conversion:

$$x = r \cdot \cos(\phi) \quad y = r \cdot \sin(\phi)$$

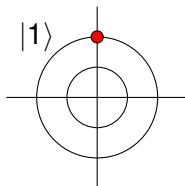
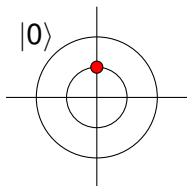
$$r = \sqrt{x^2 + y^2} \quad \phi = \arctan\left(\frac{y}{x}\right)$$

Another representation:

$$(r, \phi) = r \cdot e^{i\phi} \quad e^{i\phi} = \cos(\phi) + i \sin(\phi),$$

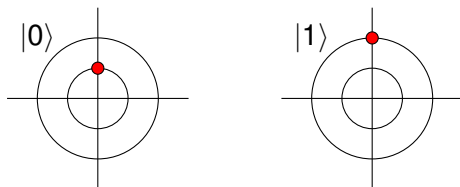
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Consider a simple systems with two **degrees of freedom**.



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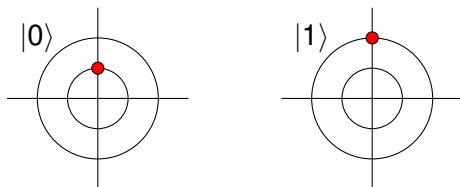
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$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$$

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Qubits live in a two-dimensional complex vector, more precisely, Hilbert space \mathbb{C}^2 and are **normalised**, i.e.

$$\| |\psi\rangle \| = \langle \psi | \psi \rangle = 1.$$

Vector Spaces

A **Vector Space** (over a field \mathbb{K} , e.g. \mathbb{R} or \mathbb{C}) is a set \mathcal{V} together with two operations:

Scalar Product $\cdot, \cdot : \mathbb{K} \times \mathcal{V} \mapsto \mathcal{V}$

Vector Addition $+, + : \mathcal{V} \times \mathcal{V} \mapsto \mathcal{V}$

such that $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{V}$ and $\alpha, \beta \in \mathbb{K}$:

1. $\mathbf{x} + (\mathbf{y} + \mathbf{z}) = (\mathbf{x} + \mathbf{y}) + \mathbf{z}$

2. $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$

3. $\exists \mathbf{o} : \mathbf{x} + \mathbf{o} = \mathbf{x}$

4. $\exists -\mathbf{x} : \mathbf{x} + (-\mathbf{x}) = \mathbf{o}$

5. $\alpha(\mathbf{x} + \mathbf{y}) = \alpha\mathbf{x} + \alpha\mathbf{y}$

6. $(\alpha + \beta)\mathbf{x} = \alpha\mathbf{x} + \beta\mathbf{x}$

7. $(\alpha\beta)\mathbf{x} = \alpha(\beta\mathbf{x})$

8. $1\mathbf{x} = \mathbf{x}$ ($1 \in \mathbb{K}$)

Tuple Spaces

Theorem

All finite dimensional vector spaces are isomorphic to the (finite) Cartesian product of the underlying field \mathbb{K}^n (i.e. \mathbb{R}^n or \mathbb{C}^n).

$$\vec{x} = (x_1, x_2, x_3, \dots, x_n) \text{ represents } \mathbf{x} = \sum_{i=1}^n x_i \mathbf{b}_i$$

$$\vec{y} = (y_1, y_2, y_3, \dots, y_n) \text{ represents } \mathbf{y} = \sum_{i=1}^n y_i \mathbf{b}_i$$

Finite dimensional vectors can be represented as tuples via their coordinates with respect to a base $\{\mathbf{b}_i\}_{i=1}^n$.

$$\alpha \vec{x} = (\alpha x_1, \alpha x_2, \alpha x_3, \dots, \alpha x_n)$$

$$\vec{x} + \vec{y} = (x_1 + y_1, x_2 + y_2, x_3 + y_3, \dots, x_n + y_n)$$

Hilbert Spaces

A complex vector space \mathcal{H} is called an **Inner Product Space** or **(Pre-)Hilbert Space** if there is a complex valued function $\langle \cdot, \cdot \rangle$ on $\mathcal{H} \times \mathcal{H}$ that satisfies $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{H}$ and $\forall \alpha \in \mathbb{C}$:

1. $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$
2. $\langle \mathbf{x}, \mathbf{x} \rangle = 0 \iff \mathbf{x} = \mathbf{o}$
3. $\langle \alpha \mathbf{x}, \mathbf{y} \rangle = \alpha \langle \mathbf{x}, \mathbf{y} \rangle$
4. $\langle \mathbf{x} + \mathbf{y}, \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{z} \rangle + \langle \mathbf{y}, \mathbf{z} \rangle$
5. $\langle \mathbf{x}, \mathbf{y} \rangle = \overline{\langle \mathbf{y}, \mathbf{x} \rangle}$

The function $\langle \cdot, \cdot \rangle$ is called an **inner product** on \mathcal{H} .

Caveat: Linear in first or second argument?

Mathematical Convention:

$$\langle \alpha \mathbf{x}, \mathbf{y} \rangle = \alpha \langle \mathbf{x}, \mathbf{y} \rangle$$

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For physicists it is simply:

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Basis Vectors

A set of vectors \mathbf{x}_i is said to be **linearly independent** iff

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An **orthonormal** system in a Hilbert space is a set of linearly independent set of vectors with:

$$\langle \mathbf{b}_i, \mathbf{b}_j \rangle = \delta_{ij} = \begin{cases} 1 & \text{iff } i = j \\ 0 & \text{iff } i \neq j \end{cases}$$

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Theorem

For a Hilbert space there exists an orthonormal basis $\{\mathbf{b}\}$. The representation of each vector is unique:

$$\mathbf{x} = \sum_i x_i \mathbf{b}_i = \sum_i \langle \mathbf{x}, \mathbf{b}_i \rangle \mathbf{b}_i$$

The Finite-Dimensional Hilbert Spaces \mathbb{C}^n

We represent vectors and their **transpose** using coordinates:

$$\vec{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = |x\rangle, \quad \vec{y} = (y_1, \dots, y_n) = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}^T = \langle y|$$

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We can also define a **norm** (length) $\|\vec{x}\| = \sqrt{\langle \vec{x}, \vec{x} \rangle}$.

Dual and Adjoint States

A **linear functional** on a vector space \mathcal{V} is a map $f : \mathcal{V} \rightarrow \mathbb{K}$ such that (i) $f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$ and (ii) $f(\alpha\mathbf{x}) = \alpha f(\mathbf{x})$ for all $\mathbf{x}, \mathbf{y} \in \mathcal{V}, \alpha \in \mathbb{K}$.

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Theorem (Riesz Representation Theorem)

Every linear functional $f : \mathcal{H} \rightarrow \mathbb{C}$ on a Hilbert space \mathcal{H} can be represented by a vector \mathbf{y}_f in \mathcal{H} , such that

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We represent vectors or **ket-vectors** as **column** vectors; and functionals, dual vector or **bra-vectors** as **row** vectors.

Dirac Notation and Einstein Convention

We will use throughout P.A.M. Dirac's bra-(c)-ket notation:

$$\langle \mathbf{x}_i, \mathbf{y}_j \rangle = \langle \vec{x}_i, \vec{y}_j \rangle \text{ denoted as } \langle x_i | | y_j \rangle = \langle i | | j \rangle$$

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A. Einstein: If in an expression there are matching sub- and super-scripts then this implicitly indicates a summation,

$$\bar{x}_i y^i = \sum_i \bar{x}_i y^i = \langle \vec{x}, \vec{y} \rangle \text{ and } x_i y^{i*} = \sum_i x_i \bar{y}^i = \langle \vec{x} | \vec{y} \rangle$$

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We represent the **coordinates** of a qubit (state) or ket-vector as a column vector:

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \alpha|0\rangle + \beta|1\rangle$$

with respect to the (orthonormal) **basis** $\{|0\rangle, |1\rangle\}$, i.e. the so-called **standard base**:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Representing a Qubit [*]

A qubit $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$ can be represented:

$$|\psi\rangle = \cos(\theta/2) |0\rangle + e^{i\varphi} \sin(\theta/2) |1\rangle,$$

where $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi]$.

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with $r_0^2 + r_1^2 = 1$. Take $r_0 = \cos(\rho)$ and $r_1 = \sin(\rho)$ for some ρ . Set $\theta/2 = \rho$, then $|\psi\rangle = \cos(\theta/2) e^{i\phi_0} |0\rangle + \sin(\theta/2) e^{i\phi_1} |1\rangle$, with $0 \leq \theta \leq \pi$, or equivalently

$$|\psi\rangle = e^{i\gamma} (\cos(\theta/2) |0\rangle + e^{i\varphi} \sin(\theta/2) |1\rangle),$$

with $\varphi = \phi_1 - \phi_0$ and $\gamma = \phi_0$, with $0 \leq \varphi \leq 2\pi$.

Representing a Qubit [*]

A qubit $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$ can be represented:

$$|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\varphi}\sin(\theta/2)|1\rangle,$$

where $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi]$. Using polar coordinates we have:

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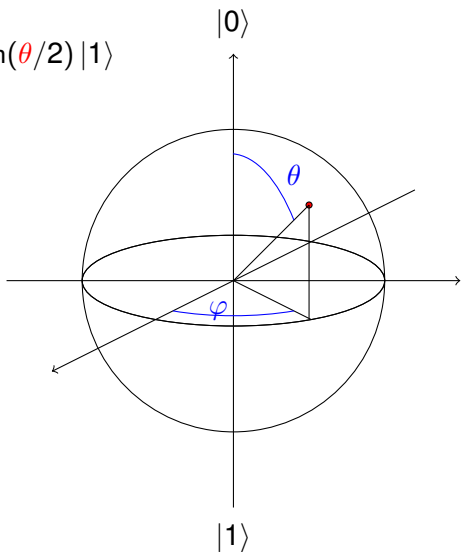
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with $\varphi = \phi_1 - \phi_0$ and $\gamma = \phi_0$, with $0 \leq \varphi \leq 2\pi$. The global **phase shift** $e^{i\gamma}$ is physically irrelevant (unobservable).

Bloch Sphere [*]

$$\cos(\theta/2) |0\rangle + e^{i\varphi} \sin(\theta/2) |1\rangle$$



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A qubit is therefore represented in the two bases as:

$$\begin{aligned} \alpha|0\rangle + \beta|1\rangle &= \frac{\alpha}{\sqrt{2}}(|+\rangle + |-\rangle) + \frac{\beta}{\sqrt{2}}(|+\rangle - |-\rangle) \\ &= \frac{\alpha + \beta}{\sqrt{2}}|+\rangle + \frac{\alpha - \beta}{\sqrt{2}}|-\rangle \end{aligned}$$

Linear Operators

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A map $\mathbf{T} : \mathcal{V} \rightarrow \mathcal{W}$ between two vector spaces \mathcal{V} and \mathcal{W} is called a **linear** map if

1. $\mathbf{T}(\mathbf{x} + \mathbf{y}) = \mathbf{T}(\mathbf{x}) + \mathbf{T}(\mathbf{y})$ and
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for all $\mathbf{x}, \mathbf{y} \in \mathcal{V}$ and all $\alpha \in \mathbb{K}$ (e.g. $\mathbb{K} = \mathbb{C}$ or \mathbb{R}).

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for all $\mathbf{x}, \mathbf{y} \in \mathcal{V}$ and all $\alpha \in \mathbb{K}$ (e.g. $\mathbb{K} = \mathbb{C}$ or \mathbb{R}).

For $\mathcal{V} = \mathcal{W}$ we talk about a **(linear) operator** on \mathcal{V} .

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then this is enough to know the T_{ij} 's to know what \mathbf{T} is doing to all vectors (as they are representable as linear combinations of the basis vectors).

Matrices

Using a “mathematical” indexing (starting from 1 rather than 0), using the first index to indicate a **row** position and second for a **column** position, we can identify **T** with a matrix:

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One can also express this, for $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ also as:

$$\mathbf{T}(|\psi\rangle) = \mathbf{T}(\alpha|0\rangle + \beta|1\rangle) = \alpha\mathbf{T}(|0\rangle) + \beta\mathbf{T}(|1\rangle) = \mathbf{T}|\psi\rangle$$

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The **application** of a linear operator \mathbf{T} (represented by a matrix) to a vector \mathbf{x} (represented via its coordinates) becomes:

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Finite-dimensional linear operators (matrices) form a vector space and with the multiplication a (linear) **algebra**. Adding the adjoint operation (see below) turns this into a **C*-algebra**.

Transformations

We can define a linear map **B** which implements the base change $\{|0\rangle, |1\rangle\}$ and $\{|+\rangle, |-\rangle\}$:

$$\mathbf{B} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

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Transforming the coordinates (x_i) with respect to $\{|0\rangle, |1\rangle\}$ into coordinates (y_i) using $\{|+\rangle, |-\rangle\}$ can be obtained by:

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Problem: It is not easy to compute **inverse** \mathbf{B}^{-1} , defined on implicitly by $\mathbf{B}\mathbf{B}^{-1} = \mathbf{B}^{-1}\mathbf{B} = \mathbf{I}$ the identity (existence?!).

Adjoint Operator

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In **mathematics** the adjoint operator is usually denoted by \mathbf{T}^* (cf. conjugate in physics) and defined implicitly via:

$$\langle \mathbf{T}(\mathbf{x}), \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{T}^*(\mathbf{y}) \rangle \quad \text{or} \quad \langle \mathbf{T}^\dagger \mathbf{x} \mid \mathbf{y} \rangle = \langle \mathbf{x} \mid \mathbf{T} \mathbf{y} \rangle$$

Adjoint Vectors

Bra and ket vectors are also related using the adjoint:

$$|x\rangle^\dagger = \langle x|$$

or using their coordinates:

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The adjoint operator specifies the effect on dual vectors:

$$(\mathbf{T}|\mathbf{x}\rangle)^\dagger = |\mathbf{x}\rangle^\dagger \mathbf{T}^\dagger = \langle \mathbf{x}| \mathbf{T}^\dagger$$

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The unitary evolution of an (isolated) quantum state/system is a mathematical consequence of being a solution of the Schrödinger equation for some Hamiltonian operator \mathbf{H} .

Properties of Unitary Operators

Unitary operators generalise in some sense permutations (in fact every permutation of base vectors gives rise to a simple unitary map). They can also be seen as generalised rotations.

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Any single qubit operation, i.e. unitary 2×2 matrix \mathbf{U} can be expressed as via 4 (real) parameters:

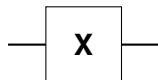
$$\mathbf{U} = \begin{pmatrix} e^{i(\alpha-\beta/2-\delta/2)} \cos \gamma/2 & e^{i(\alpha+\beta/2-\delta/2)} \sin \gamma/2 \\ -e^{i(\alpha-\beta/2+\delta/2)} \sin \gamma/2 & e^{i(\alpha+\beta/2+\delta/2)} \cos \gamma/2 \end{pmatrix}$$

where α , β , δ and γ are real numbers.

Basic 1-Qubit Operators

Pauli X-Gate

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



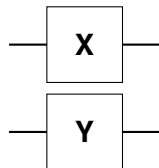
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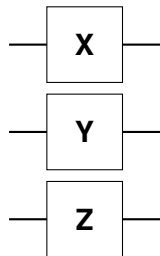
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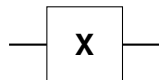
$$\mathbf{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



Basic 1-Qubit Operators

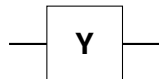
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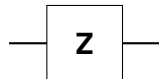
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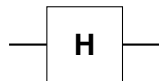
Pauli Z-Gate

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Hadamard Gate

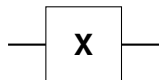
$$\mathbf{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$



Basic 1-Qubit Operators

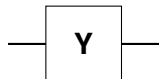
Pauli X-Gate

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



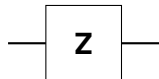
Pauli Y-Gate

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



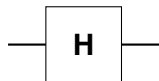
Pauli Z-Gate

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



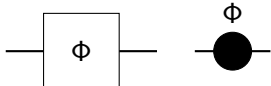
Hadamard Gate

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



Phase Gate

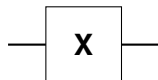
$$\Phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$



Basic 1-Qubit Operators

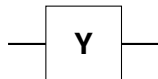
Pauli X-Gate

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



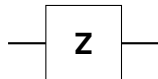
Pauli Y-Gate

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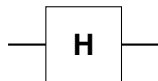
Pauli Z-Gate

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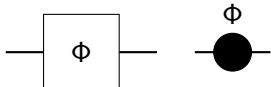
Hadamard Gate

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



Phase Gate

$$\Phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$



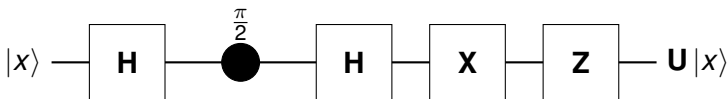
The Pauli-X gate is often referred to as NOT gate. Note that the notation for Hamiltonian and Hadamard gate are both **H**.

Graphical “Notation”

The product (combination) of unitary operators results in a unitary operator, i.e. with $\mathbf{U}_1, \dots, \mathbf{U}_n$ unitary, the product $\mathbf{U} = \mathbf{U}_n \dots \mathbf{U}_1$ is also unitary (Note: $(\mathbf{TS})^\dagger = \mathbf{S}^\dagger \mathbf{T}^\dagger$).

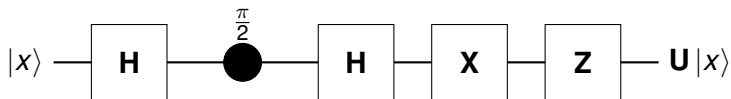
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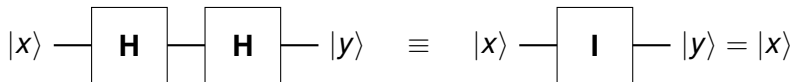


Graphical “Notation”

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A simple example: $|y\rangle = \mathbf{H}\mathbf{H}|x\rangle$ or $(|x\rangle; \mathbf{H}; \mathbf{H} = |y\rangle)$:



because $\mathbf{H}^2 = \mathbf{I}$, i.e.

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