Quantum Computation (CO484) Quantum States and Evolution

Herbert Wiklicky

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- The only possible results are eigen-values λ_i of **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 **A**.

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Complex Numbers

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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:

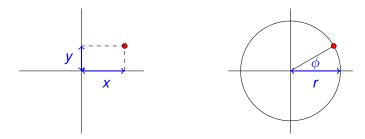
$$z^* = \overline{z} = \overline{x + iy} = x - iy = z^\dagger$$

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:

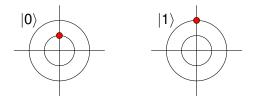
$$x = r \cdot \cos(\phi)$$
 $y = r \cdot \sin(\phi)$
 $r = \sqrt{x^2 + y^2}$ $\phi = \arctan(\frac{y}{x})$

Another representation:

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

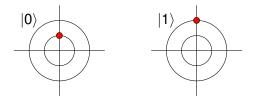
Computational Quantum States

Consider a simple systems with two degrees of freedom.



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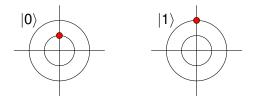
Definition A qubit (quantum bit) is a quantum state of the form

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

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$$\left|\psi\right\rangle = \alpha \left|\mathbf{0}\right\rangle + \beta \left|\mathbf{1}\right\rangle$$

where α and β are complex numbers with $|\alpha|^2 + |\beta|^2 = 1$. 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:

 $\begin{array}{l} \text{Scalar Product } \ldots \colon \mathbb{K} \times \mathcal{V} \mapsto \mathcal{V} \\ \text{Vector Addition } .+ \colon \mathcal{V} \times \mathcal{V} \mapsto \mathcal{V} \end{array}$

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

1. x + (y + z) = (x + y) + z**2.** x + y = y + x**3.** $\exists o : x + o = x$ **4**. $\exists -x : x + (-x) = o$ 5. $\alpha(\mathbf{x} + \mathbf{v}) = \alpha \mathbf{x} + \alpha \mathbf{v}$ 6. $(\alpha + \beta)\mathbf{X} = \alpha \mathbf{X} + \beta \mathbf{X}$ 7. $(\alpha\beta)\mathbf{x} = \alpha(\beta\mathbf{x})$ 8. $1x = x \ (1 \in \mathbb{K})$ イロン 不得 とくほ とくほう 一日

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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).

$$\vec{x} = (x_1, x_2, x_3, \dots, x_n)$$
 represents $\mathbf{x} = \sum_{i=1}^n x_i \mathbf{b}_i$
 $\vec{y} = (y_1, y_2, y_3, \dots, y_n)$ 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 $\langle ., . \rangle$ 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.
$$\langle \mathbf{x}, \mathbf{x} \rangle \ge 0$$

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

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

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$$\langle \mathbf{x} \mid \boldsymbol{\alpha} \mathbf{y} \rangle = \boldsymbol{\alpha} \langle \mathbf{x} \mid \mathbf{y} \rangle$$

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For physicists it is simply:

$$\langle \mathbf{x} \mid \alpha \mathbf{y} \rangle = \boldsymbol{\alpha} \langle \mathbf{x} \mid \mathbf{y} \rangle$$

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 $\{b\}$. The representation of each vector is unique:

$$\mathbf{x} = \sum_{i} x_{i} \mathbf{b}_{i} = \sum_{i} \langle \mathbf{x}, \mathbf{b}_{i} \rangle \mathbf{b}_{i}$$

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) $\|\vec{x}\| = \sqrt{\langle \vec{x}, \vec{x} \rangle}$.

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A linear functional on a vector space \mathcal{V} is a map $f : \mathcal{V} \to \mathbb{K}$ 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 $f : \mathcal{H} \to \mathbb{C}$ on a Hilbert space \mathcal{H} can be represented by a vector \mathbf{y}_f in \mathcal{H} , such that

$$f(\mathbf{x}) = \langle \mathbf{y}_f, \mathbf{x} \rangle = f_y(\mathbf{x})$$

Dual Hilbert spaces \mathcal{H}^* are isomorphic to the original Hilbert space \mathcal{H}^* ; in particular we have: $(\mathbb{C}^n)^* = \mathbb{C}^n$.

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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:

 $\langle \mathbf{x}_{i}, \mathbf{y}_{j} \rangle = \langle \vec{x}_{i}, \vec{y}_{j} \rangle$ 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 implicitely indicates a summation,

$$ar{x}_i y^i = \sum_i ar{x}_i y^i = \langle ec{x}, ec{y}
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 and $x_i y^{i*} = \sum_i x_i ec{y}^i = \langle ec{x} \mid ec{y}
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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:

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

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

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$$\left|\psi\right\rangle = r_{0}e^{i\phi_{0}}\left|0\right\rangle + r_{1}e^{i\phi_{1}}\left|1\right\rangle,$$

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$$\ket{\psi} = oldsymbol{e}^{i\gamma} (\cos(heta/2) \ket{0} + oldsymbol{e}^{iarphi} \sin(heta/2) \ket{1}),$$

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

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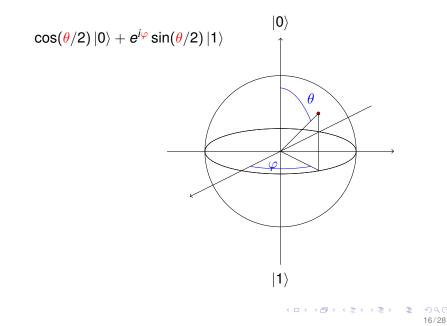
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with $r_0^2 + r_1^2 = 1$. Take $r_0 = \cos(\rho)$ and $r_1 = \sin(\rho)$ for some ρ . Set $\theta/2 = \rho$, then $|\psi\rangle = \cos(\theta/2)e^{i\phi_0}|0\rangle + \sin(\theta/2)e^{i\phi_1}|1\rangle$, with $0 \le \theta \le \pi$, or equivalently

$$\ket{\psi} = oldsymbol{e}^{i arphi}(\cos(heta/2) \ket{0} + oldsymbol{e}^{i arphi} \sin(heta/2) \ket{1}),$$

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

Bloch Sphere [*]



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A qubit is therefore represented in the two bases as:

$$\begin{array}{ll} \alpha \left| \mathbf{0} \right\rangle + \beta \left| \mathbf{1} \right\rangle &=& \displaystyle \frac{\alpha}{\sqrt{2}} (\left| + \right\rangle + \left| - \right\rangle) \frac{\beta}{\sqrt{2}} (\left| + \right\rangle - \left| - \right\rangle) \\ &=& \displaystyle \frac{\alpha + \beta}{\sqrt{2}} \left| + \right\rangle + \displaystyle \frac{\alpha - \beta}{\sqrt{2}} \left| - \right\rangle \end{array}$$

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Linear Operators

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Definition

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

1.
$$\mathbf{T}(\mathbf{x} + \mathbf{y}) = \mathbf{T}(\mathbf{x}) + \mathbf{T}(\mathbf{y})$$
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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 **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 ten 0), using the first index to indicate a **row** position and second for a **column** position, we can identify **T** with a matrix:

$$\mathbf{T} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} = (T_{ij})_{i,j=1}^n = (T_{ij})$$

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The application of **T** to a general vector (qubit) then becomes a simple matrix (pre-)multiplication:

$$\mathbf{T}\left(\left(\begin{array}{c}\alpha\\\beta\end{array}\right)\right) = \left(\begin{array}{c}T_{11} & T_{12}\\T_{21} & T_{22}\end{array}\right)\left(\begin{array}{c}\alpha\\\beta\end{array}\right) = \left(\begin{array}{c}T_{11}\alpha + T_{12}\beta\\T_{21}\alpha + T_{22}\beta\end{array}\right)$$

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

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

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

$$\mathbf{T}(\mathbf{x}) = \mathbf{T}\mathbf{x} = (T_{ij})(x_i) = \sum_i T_{ij}x_i$$

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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**.

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

$$\mathbf{B} = \frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right)$$

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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:

$$B(x_i)_i = (y_i)_i$$
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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?!).

For a matrix $\mathbf{T} = (T_{ij})$ its transpose matrix \mathbf{T}^{T} is defined as

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$$\mathbf{T}^{\dagger} = (\mathcal{T}_{ij}^{\dagger}) = (\mathcal{T}_{ji}^{*}) \quad \text{or} \ \mathbf{T}^{\dagger} = (\mathbf{T}^{*})^{\mathcal{T}} = (\mathbf{T}^{\mathcal{T}})^{*}$$

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Note that $(\mathbf{TS})^{T} = \mathbf{S}^{T}\mathbf{T}^{T}$ and thus $(\mathbf{TS})^{\dagger} = \mathbf{S}^{\dagger}\mathbf{T}^{\dagger}$.

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

$$\langle \mathsf{T}(\mathsf{x}),\mathsf{y}
angle = \langle \mathsf{x},\mathsf{T}^*(\mathsf{y})
angle \ \, \text{or} \ \, \langle \mathsf{T}^\dagger \mathsf{x} \mid \mathsf{y}
angle = \langle \mathsf{x} \mid \mathsf{Ty}
angle$$

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:

$$(\mathbf{T} \ket{x})^{\dagger} = \ket{x}^{\dagger} \mathbf{T}^{\dagger} = \langle x \mid \mathbf{T}^{\dagger}$$

A square matrix/operator U is called unitary if

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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 **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 **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.

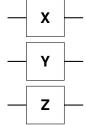
Pauli X-Gate
$$\mathbf{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
 \mathbf{X}

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

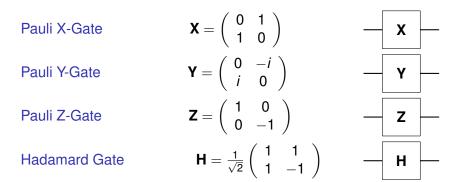


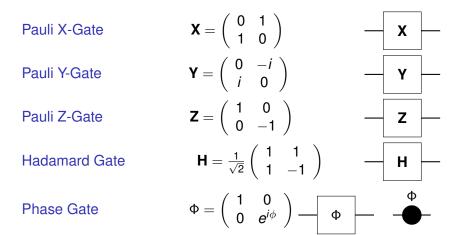
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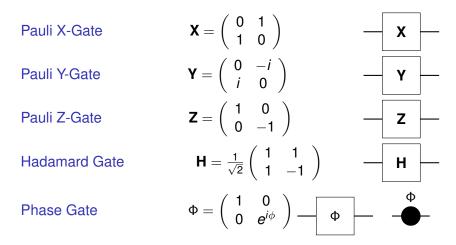
Pauli X-Gate



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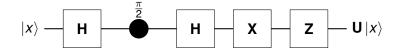
The Pauli-X gate is often referred to as NOT gate. Note that the notation for Hamiltonian and Hadamard gate are both **H**.

Graphical "Notation"

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

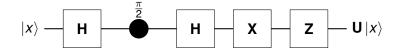
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A simple example: $|y\rangle = HH |x\rangle$ or $(|x\rangle; H; H = |y\rangle)$:

$$|x\rangle$$
 — H — $|y\rangle$ \equiv $|x\rangle$ — I — $|y\rangle = |x\rangle$

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

$$\frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right) \frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right) = \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right)$$