TryScience Workshop:
How to Program a Quantum Computer

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Prerequisites

- → Target audience: physics + math at **high-school level**
- → Required concepts:
  - Vectors (**linear algebra**)
  - Probabilities
  - Trigonometry

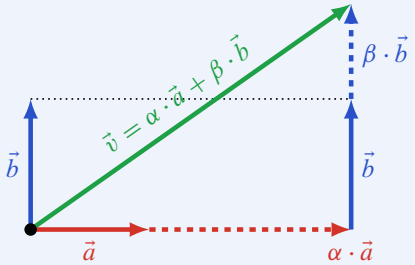
Reminder: Linear Combinations

- → Example vectors in $\mathbb{R}^2$:

$$\vec{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \in \mathbb{R}^2 \tag{1}$$

- → Linear combination (scale + add), $\alpha, \beta \in \mathbb{R}$:

$$\vec{v} = \alpha \cdot \vec{a} + \beta \cdot \vec{b} = \begin{pmatrix} \alpha\, a_1 + \beta\, b_1 \\ \alpha\, a_2 + \beta\, b_2 \end{pmatrix} \tag{2}$$



1 From Vectors to Qubits

→ ⁂ **Qubit**: elementary carrier of quantum information (cf. **bit** in a classical computer)

→ Hardware of a quantum computer: ⁂ **quantum memory** + ⁂ **quantum processor**

Example platform: ⁂ **neutral atom quantum computers**
(one atom per qubit, laser-based control)

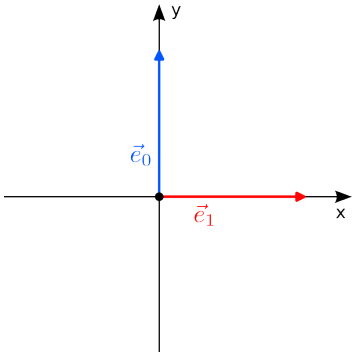
→ Programmer's view: abstract two-state system (ignore hardware details!)

→ ⁂ **Quantum information theory**

→ *"Qubits can be in two states at the same time."* → States = vectors?

Classical bit basis: two orthogonal vectors $\vec{e}_0, \vec{e}_1$:

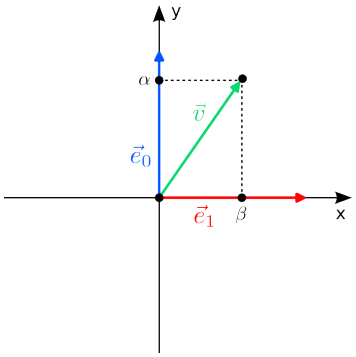
$$0 \leftrightarrow \vec{e}_0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \text{and} \qquad 1 \leftrightarrow \vec{e}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3}$$



- Basis vectors are just **labels** for two states
- Motivation: vectors allow superpositions via linear combinations

→ Superposition (linear combination):

$$\vec{v} = \alpha \cdot \vec{e}_0 + \beta \cdot \vec{e}_1 = \begin{pmatrix} \beta \\ \alpha \end{pmatrix} \tag{4}$$



- ⁂ **Amplitudes**: $\alpha, \beta \in \mathbb{R}$ (can be negative!)
- ⁂ **Basis states:**
  $(\alpha, \beta) = (1, 0) \Rightarrow \vec{v} = \vec{e}_0$
  $(\alpha, \beta) = (0, 1) \Rightarrow \vec{v} = \vec{e}_1$

→ Hypothesis: the state of a qubit is described by a 2D vector $\vec{v}$ (?)

→ Almost correct! → Constraint: ⁂ **normalization**:

$$|\vec{v}| = \sqrt{\alpha^2 + \beta^2} \stackrel{!}{=} 1 \tag{5}$$

Motivation: probability interpretation of the → *measurement* (later)

Beware: Abstract vectors

→ $\vec{v} \in \mathbb{R}^2$ is a *state vector*, not a position vector!

Neutral Atom Implementation of Qubits

→ Physical qubit: needs two internal quantum states $\vec{e}_0, \vec{e}_1$

→ Example: single ⁂ **strontium atoms**, held in traps by lasers ("optical tweezers")

→ Imaging with a microscope (fluorescence image):

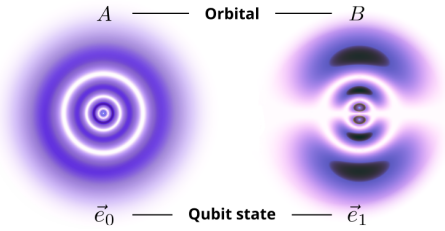


- White boxes: known trap positions (atoms can be dark → *later*)
- Each bright spot: one atom

Beware: Imaging atoms

- Atom diameter ~ 0.1 nm vs. imaging wavelength ~ 500 nm
- Optical images cannot resolve an "atom shape"

→ Basis choice: two **electronic orbitals** A and B of the atom ("electron orbits"):



- Encoding: $A \leftrightarrow \vec{e}_0$ and $B \leftrightarrow \vec{e}_1$
- Superposition: linear combinations of $\vec{e}_0, \vec{e}_1$

→ Why single atoms?

- Reduce unwanted → *measurements* by the environment (**decoherence**)
- Vacuum + microscopic systems: easier to isolate than macroscopic objects

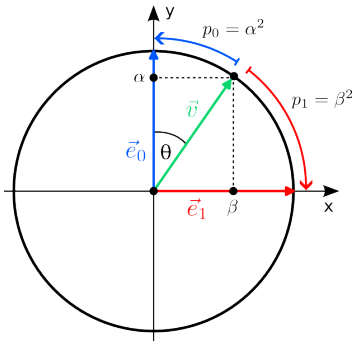
2 Measurements

→ Special feature of quantum mechanics: **measurements**

→ Outcomes: **discrete** basis states $\vec{e}_0$ or $\vec{e}_1$ (no "in between")
(Qubits are *not* tiny "compass needles"!)

→ ⁂ **Born rule**: probabilities from squared amplitudes:

$$\vec{v} = \alpha\,\vec{e}_0 + \beta\,\vec{e}_1 \xrightarrow{\text{Measurement}}$$
$$\vec{v}_{\text{new}} = \begin{cases} \vec{e}_0 & \text{with prob. } p_0 = \alpha^2 \\ \vec{e}_1 & \text{with prob. } p_1 = \beta^2 \end{cases} \tag{6}$$



State after the measurement:
⁂ **Collapse** to the observed basis state $\vec{v}_{\text{new}}$

→ Summary:

- **Quantization**: discrete outcomes from a continuous state space
- **Probabilistic**: random outcomes with state-dependent probabilities
- **Collapse**: state update to the measured basis state

→ Probability interpretation requires normalization:

$$p_0 + p_1 \overset{!}{=} 1 \quad \Leftrightarrow \quad |\vec{v}|^2 = \alpha^2 + \beta^2 \overset{!}{=} 1 \quad \Leftrightarrow \quad |\vec{v}| \overset{!}{=} 1 \tag{7}$$

→ ⁂ **Single-qubit state space** = **unit circle** (angle θ):

$$\vec{v} = \cos(\theta)\,\vec{e}_0 + \sin(\theta)\,\vec{e}_1 = \begin{pmatrix} \sin(\theta) \\ \cos(\theta) \end{pmatrix} \quad \text{for} \quad 0 \le \theta < 2\pi\,. \tag{8}$$

Reminder: $\sin^2(\theta) + \cos^2(\theta) = 1$ (automatically normalized)

→ Implication for quantum computers:
Repeat "quantum programs" many times (⁂ **shots**) to compute averages

Beware: What constitutes a measurement?

- → Measurement $\approx$ interaction that spreads **state information** into the environment
- → No conscious observer required
- → "Accidental measurements" (e.g. stray photons) $\rightarrow$ unwanted collapse (⁂ **decoherence**)
- → Engineering challenge: prevent "information leaks" (**isolation**)

3 Quantum Physics Notation

→ Common notation = ⁂ **Dirac notation**: vectors $\vec{v}$ are written as ⁂ **kets** $|\Psi\rangle$:

$$\vec{v} \mapsto |\Psi\rangle \quad \text{and} \quad \vec{e}_0 \mapsto |0\rangle \quad \text{and} \quad \vec{e}_1 \mapsto |1\rangle \ . \tag{9}$$

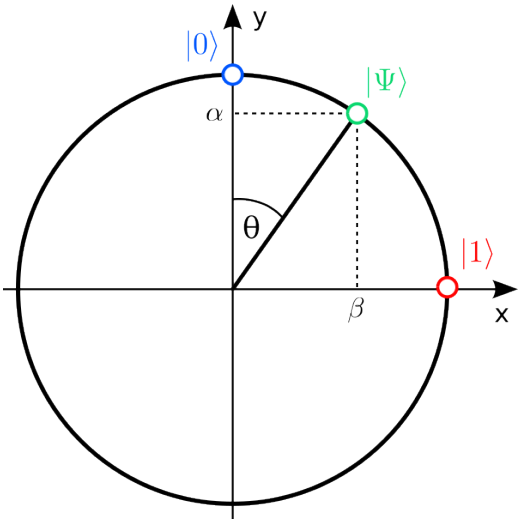
Reason: more compact formulas; easy generalization to many qubits (→ *later*)

→ Single-qubit state in Dirac notation:

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \qquad \text{with} \qquad \alpha^2 + \beta^2 = 1 \tag{10}$$

- **Amplitudes**: α, β
- **Basis kets**: $|0\rangle\,, |1\rangle$

→ State space in Dirac notation:



Beware: Quantum state vs. wave function

→ "Wave function" historically: state as a function of position

→ Qubit states $|0\rangle\,, |1\rangle$ are *not* position wave functions!

→ We use the term **quantum state**

4 Many Qubits

→ Useful quantum computers need **many qubits**

→ Questions:

- How do we describe states of many qubits?
- How many qubits are "enough"?

4.1 Quantum States of Many Qubits

→ Visualization impossible: the single-qubit circle picture does not generalize!
(But calculations with linear algebra still work!)

→ Measurement outcomes for N qubits: **bit strings** $x_1 x_2 \dots x_N$ with $x_i \in \{0, 1\}$

→ One basis ket for each classical configuration:

$$|x_1 x_2 \dots x_N\rangle \tag{11}$$

→ 2^N basis states for N qubits

→ Example $N = 2$ ($2^2 = 4$):

$$|00\rangle\,,\ |01\rangle\,,\ |10\rangle\,,\ |11\rangle \tag{12}$$

→ Dimension of the state space: 2^N (requires 2^N orthogonal basis vectors)
(Example: $N = 2 \rightarrow$ state space = $\mathbb{R}^4 \rightarrow$ cannot be visualized)

→ General state: **linear combination** of all basis states:

$$|\Psi\rangle = \alpha\,|00\rangle + \beta\,|01\rangle + \gamma\,|10\rangle + \delta\,|11\rangle \tag{13}$$

Amplitudes: $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ (in general: 2^N amplitudes)

→ Measurements: generalization of the **Born rule**:

$$|\Psi\rangle \xrightarrow{\text{Measurement}} |\Psi_{\text{new}}\rangle = \begin{cases} |00\rangle & \text{with probability } p_0 = \alpha^2 \\ |01\rangle & \text{with probability } p_1 = \beta^2 \\ |10\rangle & \text{with probability } p_2 = \gamma^2 \\ |11\rangle & \text{with probability } p_3 = \delta^2 \end{cases} \tag{14}$$

- **Probabilities**: squares of the amplitudes

- **Normalization**:

$$\alpha^2 + \beta^2 + \gamma^2 + \delta^2 \stackrel{!}{=} 1 \tag{15}$$

→ Still "vector length one" in $\mathbb{R}^{(2^N)}$

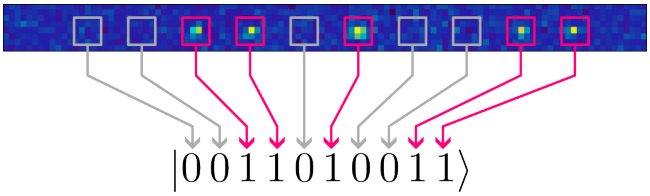
Beware: The circle picture does not generalize to many qubits!

- **Caution:** N qubits are *not* N independent points on a circle!
- Counting: 2^N amplitudes $> N$ angles

→ Example: state measurement with **neutral atoms**:

- Illuminate atoms with a laser (⁂ **state-selective fluorescence**):

  $|0\rangle$ = orbital A → stays **dark**, $|1\rangle$ = orbital B → **glows**
- Camera image → bit-string outcome:



  - Dark box ⇒ $|0\rangle$, bright box ⇒ $|1\rangle$
  - Example measurement: $|0011010011\rangle$

4.2 Classical Simulation of Quantum States

→ Classical simulation of N qubits → store 2^N **amplitudes**

→ Memory estimate: 4 bytes per real amplitude:

$$M = 2^N \times 4\,\text{byte} \quad \text{memory for the quantum state of } N \text{ qubits} \tag{16}$$

- Example: $M = 16$ GB RAM (laptop) → $N \approx 32$ qubits
- Example: $M = 1$ TB RAM (server) → $N \approx 38$ qubits
- Example: $N = 100$ qubits (= atoms) → $M = 2^{100} \times 4\,\text{byte} = 5 \times 10^{18}$ TB of memory needed

→ $N \gtrsim 50$ qubits: hard to simulate; $N \sim 100$ qubits: impossible to simulate

→ Build quantum computers to study such systems!

5 Operations on Qubits

→ Basic principle of a ⁂ **quantum algorithm** (“quantum program”):

$$\underbrace{|\Psi_{\text{initial}}\rangle = |0\ldots0\rangle}_{\text{Initialization}} \underbrace{\xrightarrow{\text{Transformation}}}_{\text{The hard part!}} |\Psi_{\text{final}}\rangle \xrightarrow{\text{Measurement}} \underbrace{\begin{cases} |0\ldots0\rangle & ? \\ |0\ldots1\rangle & ? \\ & \vdots \\ |1\ldots1\rangle & ? \end{cases}}_{\text{Results}} \tag{17}$$

- Initialization: typically $|0\ldots0\rangle$
- Transformation by ⁂ **quantum gates**: $|\Psi_{\text{initial}}\rangle \mapsto |\Psi_{\text{final}}\rangle$ (details: now!)
- Measurement: one bit string per shot

Probabilistic measurement outcomes → Repeat often (**shots**) → Estimate probabilities

5.1 Quantum Gates on Single Qubits

→ ⁂ **Quantum gate** U = transformation of a quantum state (no measurement!)

→ Define U by its action on the basis states $|0\rangle, |1\rangle$:

$$\begin{aligned} |0\rangle &\xrightarrow{U} U_{00}\cdot|0\rangle + U_{01}\cdot|1\rangle \\ |1\rangle &\xrightarrow{U} U_{10}\cdot|0\rangle + U_{11}\cdot|1\rangle \end{aligned} \tag{18}$$

→ U is specified by four real numbers U_{ij}

→ Action of U on *arbitrary superpositions* via ⁂ **linearity**:

$$\begin{aligned} |\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \xrightarrow{U} \quad & \alpha\,(U_{00}\,|0\rangle + U_{01}\,|1\rangle) + \beta\,(U_{10}\,|0\rangle + U_{11}\,|1\rangle) \\ &= \underbrace{(\alpha\,U_{00} + \beta\,U_{10})}_{\alpha'}\,|0\rangle + \underbrace{(\alpha\,U_{01} + \beta\,U_{11})}_{\beta'}\,|1\rangle \\ &= \alpha'\,|0\rangle + \beta'\,|1\rangle \\ &= |\Psi'\rangle \end{aligned} \tag{19}$$

→ New amplitudes $\alpha' = \alpha U_{00} + \beta U_{10}$ and $\beta' = \alpha U_{01} + \beta U_{11}$

→ Further condition: ⁂ **orthogonality** = U preserves the **normalization** of $|\Psi\rangle$ (we skip this here)

→ U is a combination of **rotations** and **reflections** (→ *example below*)

→ Important consequences of linearity:

- **No-cloning theorem** (quantum states cannot be copied)
- **No-communication theorem** (no communication faster than light)

Example: The Hadamard Gate

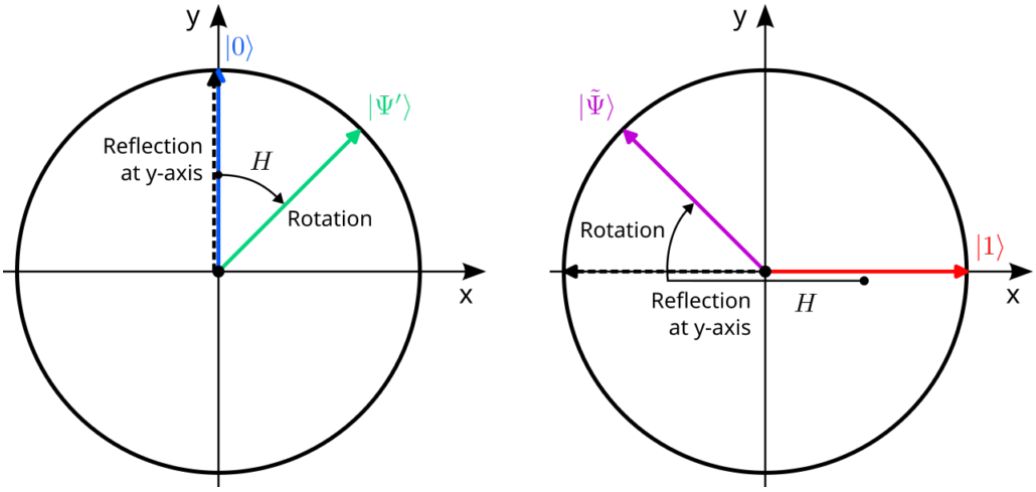
→ The ⁂ **Hadamard gate** H creates superpositions from basis states:

$$\begin{aligned} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |0\rangle \quad &\xrightarrow{H} \quad \frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |1\rangle \quad &\xrightarrow{H} \quad \frac{1}{\sqrt{2}} \cdot |0\rangle - \frac{1}{\sqrt{2}} \cdot |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} \end{aligned} \tag{20}$$

→ Four coefficients: $U_{00} = U_{01} = U_{10} = \frac{1}{\sqrt{2}}$ and $U_{11} = -\frac{1}{\sqrt{2}}$

→ Geometric interpretation (single qubit!):

Reflection at the y-axis + rotation by 45° (clockwise):



→ Reminder: rotation & reflection act on the *state space* (not on physical space!)

5.2 Combining Gates on a Single Qubit

→ Gates can be **combined** by **applying them one after another**:

$$|\Psi\rangle \xrightarrow{U_1} |\Psi'\rangle \xrightarrow{U_2} |\Psi''\rangle \ldots \tag{21}$$

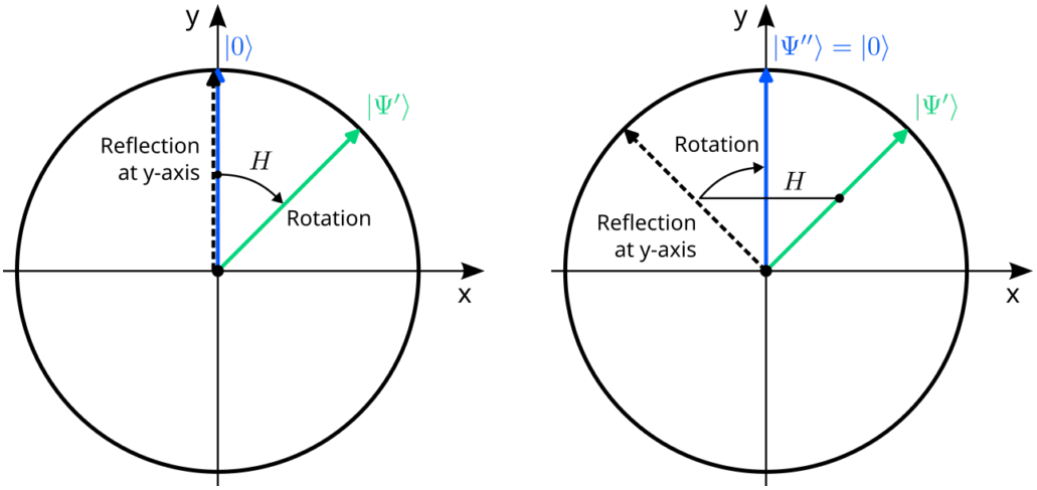
→ Goal: construct complicated gates from simple gates (LEGO principle)

Example: Combining Two Hadamard Gates

→ Goal: compute the effect of two Hadamard gates:

$$|\Psi\rangle \xrightarrow{H} |\Psi'\rangle \xrightarrow{H} |\Psi''\rangle \tag{22}$$

→ Approach 1: geometric argument (example: $|\Psi\rangle = |0\rangle$):



→ Reflection + rotation → Applying H twice "does nothing": $|\Psi\rangle = |\Psi''\rangle$

→ Approach 2: linear algebra:

- First application of H:

$$\begin{aligned} |\Psi\rangle = \alpha|0\rangle + \beta|1\rangle \xrightarrow{H} \alpha\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right) + \beta\left(\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle\right) \\ = \frac{\alpha+\beta}{\sqrt{2}}|0\rangle + \frac{\alpha-\beta}{\sqrt{2}}|1\rangle = |\Psi'\rangle \end{aligned} \tag{23}$$

- Second application of H:

$$\begin{aligned} |\Psi'\rangle \xrightarrow{H} \frac{\alpha+\beta}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right) + \frac{\alpha-\beta}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle\right) \\ = \alpha|0\rangle + \beta|1\rangle = |\Psi\rangle = |\Psi''\rangle \end{aligned} \tag{24}$$

Result: $|\Psi''\rangle = |\Psi\rangle$ for all initial states $|\Psi\rangle$ → The Hadamard gate is ⁂ **self-inverse**

Beware: Self-inverse gates

- ⁂ **Self-inverse** gates are special, not the rule!
- Example: a rotation by ϑ is self-inverse only for $\vartheta \in \{0, \pi\} \pmod{2\pi}$.

5.3 Gates on Many Qubits

→ ⁂ **Quantum algorithm** = sequence of gates on many qubits

→ Specification of ⁂ N**-qubit gates**:
Define the action on all 2^N basis states $|x_1 x_2 \dots x_N\rangle$

Example 1: The Hadamard Gate on Two Qubits

→ Hadamard gate = single-qubit gate → $N = 2$ qubits → **Two** Hadamard gates:
H_1 acts on qubit 1, H_2 on qubit 2

→ Reminder: two-qubit basis: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

→ Transformation for H_1:

$$\begin{aligned} |00\rangle &\xrightarrow{H_1} \tfrac{1}{\sqrt{2}}|00\rangle + \tfrac{1}{\sqrt{2}}|10\rangle \\ |01\rangle &\xrightarrow{H_1} \tfrac{1}{\sqrt{2}}|01\rangle + \tfrac{1}{\sqrt{2}}|11\rangle \\ |10\rangle &\xrightarrow{H_1} \tfrac{1}{\sqrt{2}}|00\rangle - \tfrac{1}{\sqrt{2}}|10\rangle \\ |11\rangle &\xrightarrow{H_1} \tfrac{1}{\sqrt{2}}|01\rangle - \tfrac{1}{\sqrt{2}}|11\rangle \end{aligned} \tag{25}$$

Note: H_1 transforms only qubit 1 (qubit 2 stays unchanged) → **Single-qubit gate**

→ Exercise: What are the transformation rules for H_2?

Example 2: The Controlled-NOT Gate

→ Example of a ⁂ **two-qubit gate** (depends on *two* qubits)

→ ⁂ **Controlled-NOT gate** (**CNOT**):
Flips one qubit (⁂ **target**) if and only if another qubit (⁂ **control**) is in $|1\rangle$
Notation: $\mathrm{CNOT}_{i \to j}$ (control i, target j)

→ Transformation for $\text{CNOT}_{1\to 2}$:

$$\begin{aligned} |00\rangle &\xrightarrow{\text{CNOT}_{1\to 2}} |00\rangle \\ |01\rangle &\xrightarrow{\text{CNOT}_{1\to 2}} |01\rangle \\ |10\rangle &\xrightarrow{\text{CNOT}_{1\to 2}} |11\rangle \\ |11\rangle &\xrightarrow{\text{CNOT}_{1\to 2}} |10\rangle \end{aligned} \tag{26}$$

Note: qubit 1 (control) unchanged; qubit 2 (target) flipped only if control is $|1\rangle$

→ Exercise: What are the rules for $\text{CNOT}_{2\to 1}$?

5.4 Many Gates on Many Qubits: A Simple Quantum Algorithm

→ Two-qubit initial state: $|\Psi_0\rangle = |00\rangle$

→ Goal: chain **two gates** on **two qubits**: first H_1, then $\text{CNOT}_{1\to 2}$

- Step 1: apply H_1:

$$|\Psi_0\rangle = |00\rangle \xrightarrow{H_1} \tfrac{1}{\sqrt{2}}|00\rangle + \tfrac{1}{\sqrt{2}}|10\rangle = |\Psi_1\rangle \tag{27}$$

- Step 2: apply $\text{CNOT}_{1\to 2}$ (**linearity**!):

$$|\Psi_1\rangle \xrightarrow{\text{CNOT}_{1\to 2}} \tfrac{1}{\sqrt{2}}|00\rangle + \tfrac{1}{\sqrt{2}}|11\rangle = |\Psi_2\rangle \tag{28}$$

→ Special final state $|\Psi_2\rangle$: ⁂ **Bell state** (also called ⁂ **EPR pair**)

→ Why special? Measure $|\Psi_2\rangle$ (**Born rule**):

$$|\Psi_2\rangle = \tfrac{1}{\sqrt{2}}|00\rangle + \tfrac{1}{\sqrt{2}}|11\rangle \xrightarrow{\text{Measurement}} |\Psi_3\rangle = \begin{cases} |00\rangle & \text{with } p_0 = 0.5 \\ |01\rangle & \text{with } p_1 = 0 \\ |10\rangle & \text{with } p_2 = 0 \\ |11\rangle & \text{with } p_3 = 0.5 \end{cases} \tag{29}$$

- Observable outcomes: only $|00\rangle$ or $|11\rangle$ (each with probability $1/2$)
- Random outcomes for each qubit, but perfectly ⁂ **correlated**!

  → ⁂ **Quantum entanglement** between qubits 1 and 2

→ **Quantum entanglement** = correlation between qubit pairs that is *stronger* than classically possible (Experimentally testable via ⁂ **Bell tests**)