

Lecture 2: Qubit Representations, Rotation Gates, and Variational Circuits

with Postulates of Quantum Mechanics and a Trainable Single-Qubit Model

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Lecture Overview

1. Vector basics – basis vectors, inner product, norm
 2. Postulates of Quantum Mechanics – state space, evolution, measurement (Born rule), composite systems
 3. Qubit state on the Bloch sphere – angles θ and φ
 4. Rotation gates – how they change the qubit state
 5. Python simulation with PennyLane & PyTorch – visualizing rotations, train-test split
 6. Application: single-qubit predictor for $\sin(x)$ – a first variational quantum circuit with proper evaluation
 7. Multi-qubit systems – tensor products, entanglement
 8. Why unitary? – from Schrödinger equation to quantum gates
 9. Summary and next lecture
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Vector Basics for Quantum States

A quantum state is a vector in a complex vector space.

For a single qubit, the space is \mathbb{C}^2 (two-dimensional complex space).

Basis vectors

Any vector can be written as a combination of basis vectors.

The **computational basis** is:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

A general qubit state is:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \quad \alpha, \beta \in \mathbb{C}.$$

Inner product and norm

The inner product $\langle\phi|\psi\rangle$ is the dot product with complex conjugation:

$$\langle\phi|\psi\rangle = \phi^*\psi_0 + \phi^*\psi_1.$$

The **norm** of a vector is $\|\psi\| = \sqrt{\langle\psi|\psi\rangle}$.

For a valid quantum state we require **normalization**: $\|\psi\| = 1$, i.e.

$$|\alpha|^2 + |\beta|^2 = 1.$$

Postulates of Quantum Mechanics

To understand how qubits behave, we need the fundamental rules

- the **postulates of quantum mechanics**.

They are stated here in the simplified form suitable for finite-dimensional systems.

Postulate 1: State Space

The state of an isolated physical system is represented by a **unit vector** in a complex Hilbert space (inner product space).

For a qubit, this space is \mathbb{C}^2 .

Postulate 2: Evolution

The evolution of a closed quantum system is described by a **unitary transformation**.

If the state at time t_1 is $|\psi\rangle$, then at time t_2 it is $|\psi'\rangle = U|\psi\rangle$, where U is unitary ($U^\dagger U = I$).

(Continuous time evolution is given by the Schrödinger equation, but for circuits we work with discrete gates.)

Postulate 3: Measurement (Born Rule)

Quantum measurements are described by a set of **measurement operators** $\{M_m\}$ acting on the state space. The index m refers to the measurement outcome.

If the state is $|\psi\rangle$ before measurement, the probability that result m occurs is

$$p(m) = \langle\psi|M_m^\dagger M_m|\psi\rangle,$$

and the state after measurement collapses to

$$\frac{M_m|\psi\rangle}{\sqrt{p(m)}}.$$

For a **projective measurement** in the computational basis $\{|0\rangle, |1\rangle\}$, the operators are $M_0 = |0\rangle\langle 0|$, $M_1 = |1\rangle\langle 1|$. Then

$$p(0) = |\langle 0|\psi\rangle|^2 = |\alpha|^2, \quad p(1) = |\langle 1|\psi\rangle|^2 = |\beta|^2,$$

and after measuring 0 the state becomes $|0\rangle$ (similarly for 1).

This is the **Born rule**: the probability of an outcome is the squared magnitude of the amplitude.

Postulate 4: Composite Systems

The state space of a composite physical system is the **tensor product** of the state spaces of the individual components.

For two qubits, the space is $\mathbb{C}^2 \otimes \mathbb{C}^2 \cong \mathbb{C}^4$. If one qubit is in state $|\psi_1\rangle$ and the other in $|\psi_2\rangle$, the joint state is $|\psi_1\rangle \otimes |\psi_2\rangle$ (often written $|\psi_1\psi_2\rangle$).

Not all states are product states – those that aren't are called **entangled**.

These postulates are the foundation for everything that follows.

3. The Bloch Sphere Representation

Because $|\alpha|^2 + |\beta|^2 = 1$, we can write

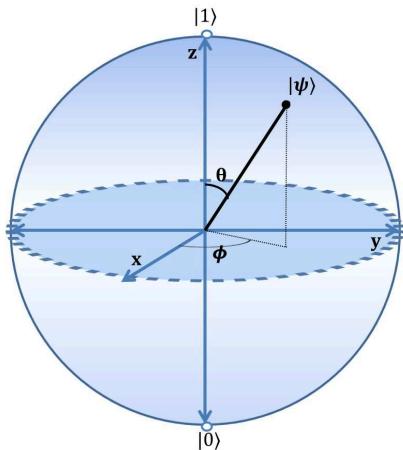
$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle,$$

with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$.

(We omit an overall global phase, which is physically unobservable.)

These two angles describe a point on the surface of a sphere – the **Bloch sphere**.

- θ (polar angle) determines the probability of measuring $|0\rangle$ vs $|1\rangle$.
- ϕ (azimuthal angle) is a relative phase.



Examples:

- $|0\rangle$: $\theta=0 \rightarrow$ north pole
 - $|1\rangle$: $\theta=\pi \rightarrow$ south pole
 - **edit**: the image shows opposite, it should be $|0\rangle$ on the up
 - $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$: $\theta=\pi/2, \phi=0 \rightarrow$ point on x-axis
 - $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$: $\theta=\pi/2, \phi=\pi \rightarrow$ opposite x-axis
 - $|+i\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$: $\theta=\pi/2, \phi=\pi/2 \rightarrow$ y-axis
-

4. Rotation Gates

Quantum gates are **unitary matrices**: $U^\dagger U = I$.

For a single qubit, rotations around the x, y, and z axes are especially important.

$$R_x(\theta) = e^{-i\frac{\theta}{2}X} = \cos \frac{\theta}{2}I - i \sin \frac{\theta}{2}X = \begin{bmatrix} \cos \frac{\theta}{2} & -i \sin \frac{\theta}{2} \\ -i \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix}$$
$$R_y(\theta) = e^{-i\frac{\theta}{2}Y} = \begin{bmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix}$$
$$R_z(\theta) = e^{-i\frac{\theta}{2}Z} = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$

Here X, Y, Z are the Pauli matrices:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Effect on the Bloch sphere

- $R_x(\theta)$ rotates the state by angle θ **around the x-axis**.
- $R_y(\theta)$ rotates around the y-axis.
- $R_z(\theta)$ rotates around the z-axis (changes only the phase φ).

For example, $R_y(\theta)$ takes $|0\rangle$ to $\cos \frac{\theta}{2}|0\rangle + \sin \frac{\theta}{2}|1\rangle$ – a superposition whose amplitudes are controlled by θ .

Simulating Rotations with PennyLane and PyTorch

We'll use **PennyLane** – a library for differentiable quantum programming – together with **PyTorch** for automatic differentiation.

```
import pennylane as qml
import torch
import matplotlib.pyplot as plt

# Create a device (simulator)
dev = qml.device('default.qubit', wires=1)

# Define a quantum function that applies a rotation and returns the expectation value of PauliZ
@qml.qnode(dev, interface='torch', diff_method='backprop')
def rotate_and_measure(theta, phi):
    qml.RY(theta, wires=0)           # rotate around y-axis
    qml.RZ(phi, wires=0)            # rotate around z-axis
    return qml.expval(qml.PauliZ(0)) # ⟨Z⟩ = probability difference

# Test with some values
theta = torch.tensor(1.2, requires_grad=True)
phi   = torch.tensor(0.5, requires_grad=True)

z_exp = rotate_and_measure(theta, phi)
print(f"Expectation value (Z) = {z_exp.item():.4f}")
```

Explanation:

- `@qml.qnode` converts the quantum function into a PennyLane **QNode** that can be executed.
- We measure the expectation value of PauliZ, which equals $P(0) - P(1)$.
- The `interface='torch'` allows us to backpropagate through the circuit.

Visualizing the effect of rotation

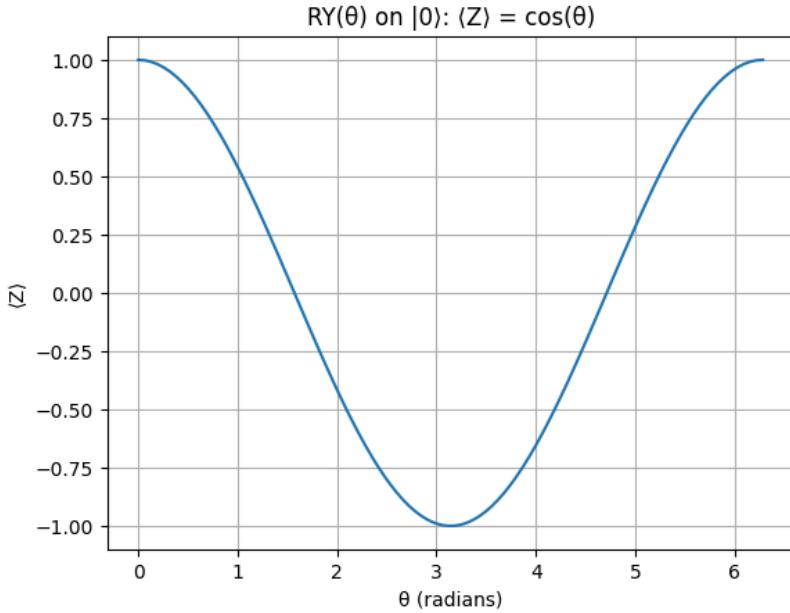
We can sweep the rotation angle and see how $\langle Z \rangle$ changes:

```

angles = torch.linspace(0, 2*torch.pi, 100)
exp_vals = [rotate_and_measure(a, 0.0) for a in angles]

plt.plot(angles.detach().numpy(), [v.item() for v in exp_vals])
plt.xlabel('θ (radians)')
plt.ylabel('⟨Z⟩')
plt.title('RY(θ) on |0⟩: ⟨Z⟩ = cos(θ)')
plt.grid()
plt.show()

```



The plot shows $\langle Z \rangle = \cos(\theta)$, exactly as expected from theory.

Application: Single-Qubit Predictor for $\sin(x)$ with Train/Test Split

Can we learn the function $f(x) = \sin(x)$ using a single qubit circuit.

- Given some x, y values
 - Can we design a model that predicts y for a given x value.
-

The idea: use a parameterized rotation to encode the input x , then train a few parameters so that the measurement output matches $\sin(x)$.

Circuit design

1. Start in $|0\rangle$.
 2. Apply $R_y(x)$ to encode the input x (this creates a state whose amplitudes depend on x).
 3. Apply a trainable rotation $R_y(\theta)$ (or a combination of rotations) – these are our **weights**.
 4. Measure $\langle Z \rangle$, which gives a value in $[-1,1]$.
 5. Compare with $\sin(x)$ (scaled to $[-1,1]$) and optimize θ .
-

We will:

- Generate synthetic data ($x, \sin(x)$).
- Split into training (80%) and test (20%) sets using `sklearn`.
- Train the model on the training set.

- Evaluate final loss on the test set.

```

import pennylane as qml
import torch
import torch.nn as nn
import torch.optim as optim
from sklearn.model_selection import train_test_split
import numpy as np
import matplotlib.pyplot as plt

class SingleQubitPredictor(nn.Module):
    def __init__(self):
        super().__init__()
        # Three trainable parameters (float32 by default)
        self.theta_z = nn.Parameter(torch.tensor(0.0))
        self.theta_y = nn.Parameter(torch.tensor(0.0))
        self.theta_x = nn.Parameter(torch.tensor(0.0))

        self.dev = qml.device('default.qubit', wires=1)

    @qml.qnode(self.dev, interface='torch', diff_method='backprop')
    def circuit(x_val, tz, ty, tx):
        qml.RY(x_val, wires=0)           # data encoding
        qml.RZ(tz, wires=0)             # trainable rotation around z
        qml.RY(ty, wires=0)             # trainable rotation around y
        qml.RX(tx, wires=0)             # trainable rotation around x
        return qml.expval(qml.PauliZ(0))

    self.circuit = circuit

    def forward(self, x):
        # x is a batch of input values (float32)
        # Call circuit for each element and convert output to float32
        preds = torch.stack([self.circuit(xi, self.theta_z, self.theta_y, self.theta_x).float() for xi in x])
        return preds

# Generate dataset (float32)
x_all = torch.linspace(-torch.pi, torch.pi, 200, dtype=torch.float32)
y_all = torch.sin(x_all)

# Train/test split
x_np = x_all.numpy().reshape(-1, 1)
y_np = y_all.numpy()
x_train_np, x_test_np, y_train_np, y_test_np = train_test_split(
    x_np, y_np, test_size=0.2, shuffle=True, random_state=42
)

x_train = torch.tensor(x_train_np.flatten(), dtype=torch.float32)
y_train = torch.tensor(y_train_np, dtype=torch.float32)
x_test = torch.tensor(x_test_np.flatten(), dtype=torch.float32)
y_test = torch.tensor(y_test_np, dtype=torch.float32)

model = SingleQubitPredictor()
optimizer = optim.Adam(model.parameters(), lr=0.1)
loss_fn = nn.MSELoss()

train_losses = []
test_losses = []

for epoch in range(50):
    # Training
    model.train()
    optimizer.zero_grad()
    y_pred_train = model(x_train)
    loss_train = loss_fn(y_pred_train, y_train)
    loss_train.backward()
    optimizer.step()
    train_losses.append(loss_train.item())

```

```

# Evaluation
model.eval()
with torch.no_grad():
    y_pred_test = model(x_test)
    loss_test = loss_fn(y_pred_test, y_test)
    test_losses.append(loss_test.item())

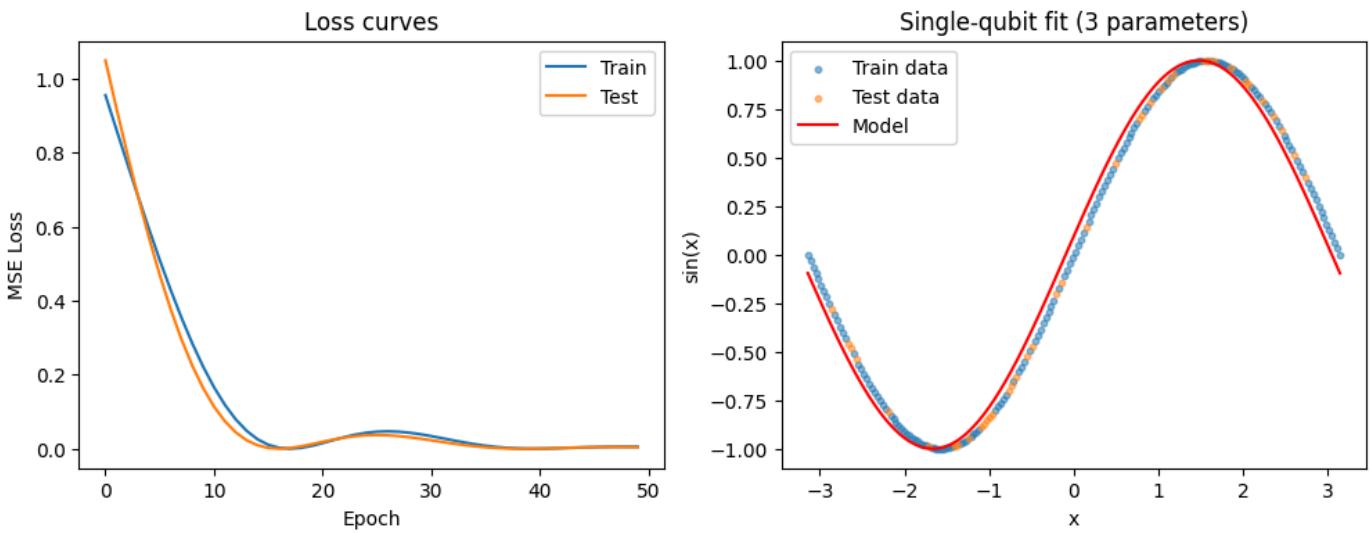
if epoch % 1 == 0:
    print(f"Epoch {epoch:3d} | Train loss: {loss_train.item():.6f} | Test loss: {loss_test.item():.6f}")

# Plotting
plt.figure(figsize=(12, 4))
plt.subplot(1, 2, 1)
plt.plot(train_losses, label='Train')
plt.plot(test_losses, label='Test')
plt.xlabel('Epoch')
plt.ylabel('MSE Loss')
plt.legend()
plt.title('Loss curves')

plt.subplot(1, 2, 2)
plt.scatter(x_train.numpy(), y_train.numpy(), s=10, alpha=0.5, label='Train data')
plt.scatter(x_test.numpy(), y_test.numpy(), s=10, alpha=0.5, label='Test data')
x_plot = torch.linspace(-torch.pi, torch.pi, 300, dtype=torch.float32)
with torch.no_grad():
    y_plot = model(x_plot)
plt.plot(x_plot.numpy(), y_plot.numpy(), 'r-', label='Model')
plt.xlabel('x')
plt.ylabel('sin(x)')
plt.legend()
plt.title('Single-qubit fit (3 parameters)')
plt.show()

print(f"Final test loss: {test_losses[-1]:.6f}")
print(f"Trained parameters: θ_z = {model.theta_z.item():.4f}, θ_y = {model.theta_y.item():.4f}, θ_x = {model.theta_x.item():.4f}")

```



What happens?

With three trainable parameters $(\theta_z, \theta_y, \theta_x)$, the circuit can implement **any single-qubit unitary**.

The circuit applies the following operations:

0. the initial state $|0\rangle$
 1. **Data encoding:** $R_Y(x)$ – rotates around the Y-axis by an angle equal to the input value x .
 2. **Trainable rotations:** $R_Z(\theta_z)$, $R_Y(\theta_y)$, $R_X(\theta_x)$ – in that order.
 3. **Measurement:** expectation value of the PauliZ operator.
-

The overall unitary is $U = R_X(\theta_x)R_Y(\theta_y)R_Z(\theta_z)R_Y(x)$, and the output is

$$f(x) = \langle 0 | R_Y(x)^\dagger R_Z(\theta_z)^\dagger R_Y(\theta_y)^\dagger R_X(\theta_x)^\dagger Z R_X(\theta_x)R_Y(\theta_y)R_Z(\theta_z)R_Y(x) | 0 \rangle.$$

Define the trainable part as $V = R_X(\theta_x)R_Y(\theta_y)R_Z(\theta_z)$. Then

$$f(x) = \langle 0 | R_Y(x)^\dagger (V^\dagger Z V) R_Y(x) | 0 \rangle.$$

This example illustrates:

- **Data encoding** into quantum states.
- **Parameterized quantum circuits** (the basis of variational quantum algorithms).
- **Training** using automatic differentiation.
- **Proper evaluation** with train/test split.

How to analyze the circuit further?

Pauli Matrices

The Pauli matrices are a set of three 2×2 complex matrices that are fundamental in quantum mechanics and quantum computing.

- They are Hermitian, unitary, and traceless, and they form a basis for the space of 2×2 Hermitian matrices.
 - They are usually denoted by σ_x , σ_y , and σ_z (or sometimes X , Y , Z).
-

1. Pauli-X (σ_x) – The "bit-flip" matrix

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

- It swaps the $|0\rangle$ and $|1\rangle$ states.
 - Eigenvalues: $+1$ (eigenvector $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$) and -1 (eigenvector $\frac{|0\rangle-|1\rangle}{\sqrt{2}}$).
-

2. Pauli-Y (σ_y) – The "bit-flip + phase-flip" matrix

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

- It applies a combination of a bit-flip and a phase-flip.
 - Eigenvalues: $+1$ (eigenvector $\frac{|0\rangle-i|1\rangle}{\sqrt{2}}$) and -1 (eigenvector $\frac{|0\rangle+i|1\rangle}{\sqrt{2}}$).
-

3. Pauli-Z (σ_z) – The "phase-flip" matrix

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

- It leaves $|0\rangle$ unchanged and flips the sign of $|1\rangle$.
 - Eigenvalues: $+1$ (eigenvector $|0\rangle$) and -1 (eigenvector $|1\rangle$).
-

Key Properties (relevant to our previous example)

1. **Hermitian:** $\sigma_i^\dagger = \sigma_i$ (they are equal to their own conjugate transpose).

2. **Traceless:** $\text{tr}(\sigma_i) = 0$.

3. **Square to Identity:** $\sigma_i^2 = I$ (the 2×2 identity matrix).

4. **Orthogonality:** $\text{tr}(\sigma_i \sigma_j) = 2\delta_{ij}$ (they are orthogonal under the trace inner product).

5. **Basis for Hermitian matrices:** Any 2×2 Hermitian matrix H can be written uniquely as

$$H = \alpha_0 I + \alpha_x \sigma_x + \alpha_y \sigma_y + \alpha_z \sigma_z$$

with real coefficients $\alpha_0, \alpha_x, \alpha_y, \alpha_z$.

In our circuit analysis, The operator $O = V^\dagger Z V$ is obtained by conjugating the Pauli-Z matrix with a unitary V .

This operation preserves two key properties of Z :

- Hermitian (property 1)
 - and traceless (property 2),
so it can be expanded as a linear combination of $\sigma_x, \sigma_y, \sigma_z$ with real coefficients.
-

Any 2×2 Hermitian traceless matrix can be expanded uniquely in the basis of the three Pauli matrices $\{\sigma_x, \sigma_y, \sigma_z\}$ with **real coefficients**.

$$O = a \sigma_x + b \sigma_y + c \sigma_z, \quad a, b, c \in \mathbb{R}.$$

because Z has eigenvalues $+1$ and -1 , its unitary conjugate O also has eigenvalues $+1$ and -1 . For a matrix of the form $a\sigma_x + b\sigma_y + c\sigma_z$, the eigenvalues are $\pm\sqrt{a^2 + b^2 + c^2}$.

For these to be ± 1 , we must have

$$\sqrt{a^2 + b^2 + c^2} = 1 \implies a^2 + b^2 + c^2 = 1.$$

- O is a genuine Pauli operator (a point on the Bloch sphere).
-

The operator $O = V^\dagger Z V$ is a Pauli operator rotated by V , so it can be written as

$$O = a\sigma_x + b\sigma_y + c\sigma_z, \quad \text{with } a^2 + b^2 + c^2 = 1.$$

Now, $R_Y(x)^\dagger O R_Y(x)$ rotates O about the Y-axis by $-x$. Using standard rotation formulas, we get

$$R_Y(-x)OR_Y(x) = (a \cos x + c \sin x)\sigma_x + b\sigma_y + (-a \sin x + c \cos x)\sigma_z.$$

Since $\langle 0|\sigma_x|0\rangle = \langle 0|\sigma_y|0\rangle = 0$ and $\langle 0|\sigma_z|0\rangle = 1$, the final output simplifies to

$$f(x) = -a \sin x + c \cos x.$$

Thus the model can only represent functions of the form

$$f(x) = A \cos x + B \sin x, \quad \text{with } A = c, B = -a,$$

and the constraint $A^2 + B^2 = a^2 + c^2 \leq 1$ (because $b^2 = 1 - a^2 - c^2 \geq 0$).

Moving to Multiple Qubits

Real quantum computers use many qubits. The state of **n qubits** lives in the tensor product space:

$$\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2 \quad (\text{n times})$$

Dimension = 2^n . A basis is given by all n-bit strings, e.g. for two qubits:

$$|00\rangle, |01\rangle, |10\rangle, |11\rangle.$$

A general two-qubit state is

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle,$$

with $\sum |\alpha_{ij}|^2 = 1$.

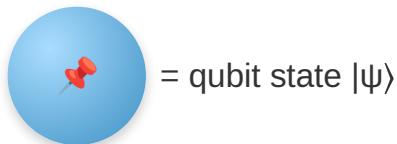
Entanglement

Some states cannot be written as a product of single-qubit states. Example:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

This is an **entangled** state – measuring one qubit instantly affects the other.

Analogy: The Quantum State as a Bubble



Think of a qubit's quantum state as a soap bubble floating in air

- The **bubble itself** = the entire quantum state (the wave function)
 - The **air inside** = the probability amplitudes (α, β)
 - The **bubble's surface** = the connection between all possible outcomes
-



Key Insight:

Just as a bubble is a single, coherent object that fills a region of space, a quantum state is a single mathematical object that encodes all possibilities for the qubit.

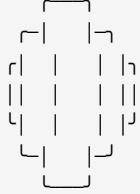
Superposition – The Bubble Is Everywhere at Once

Before Measurement: The Bubble Spreads Out



Superposition: amplitudes spread

A bubble isn't "mostly here" or "mostly there" – it's a continuous film

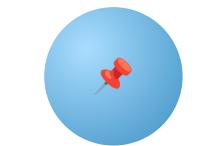


- The bubble's shape represents how the amplitudes are distributed
- You cannot point to one spot and say "the bubble is here"
- Similarly, a qubit in superposition isn't "partly $|0\rangle$ and partly $|1\rangle$ " – it's a single state with amplitude spread across basis states

Question: Where exactly is the bubble?

Answer: It's everywhere its film exists – just like a superposition state exists in all basis states simultaneously.

Measurement – Popping the Bubble



Before measurement

After measurement (collapsed)

When you pop a bubble with a pin:

- The bubble *collapses* instantly
- The air rushes out, the film disappears
- All that remains is a single tiny droplet at one random point

After Measurement: Collapse to a Single Outcome

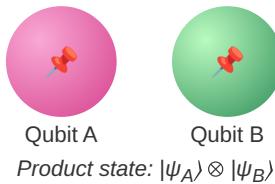


This is quantum measurement:

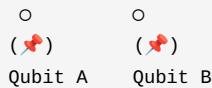
- The bubble (quantum state) collapses
- One outcome (droplet) appears randomly
- The probability of where the droplet lands follows the Born rule:
More "bubble film" in a region = higher chance the droplet appears there

Born rule visualized: The droplet is most likely to land where the bubble was "thickest" (largest amplitude).

Multiple Qubits – Bubbles Multiply



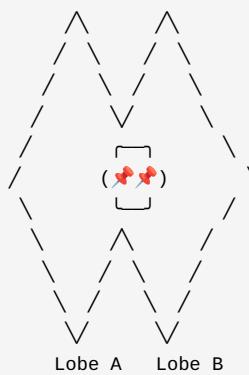
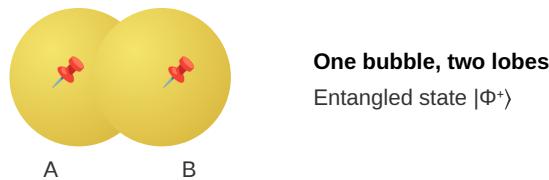
Two Unentangled Qubits = Two Separate Bubbles



- Each bubble floats independently
- Each has its own shape, its own amplitudes
- The joint state is just "bubble A AND bubble B" – a product state
- Popping bubble A affects only qubit A; bubble B remains unchanged

Mathematically: $|\psi_A\rangle \otimes |\psi_B\rangle$

Two Entangled Qubits = One Bubble with Two Lobes



This is a single bubble with two connected lobes

- The two lobes are still distinguishable (we can label them A and B)
- But they share the same film – they are part of **one unified structure**
- You cannot describe one lobe independently without reference to the other

What happens when you pop one lobe?



Popping lobe A →

The ENTIRE bubble collapses!

Two droplets appear:

↙ at A ↙ at B

Their positions are PERFECTLY CORRELATED

This is entanglement:

- The qubits remain separate physical systems (two lobes)
- But their joint state is a single entity (one connected bubble)
- Measurement affects both instantly, with correlated outcomes

| Concept | Bubble Picture | Key Idea |
|--------------------|---|---------------------------------------|
| Single qubit state |  | One coherent object |
| Superposition |  | Amplitude spread |
| Measurement |  | Collapse to one outcome |
| Product state |  | Independent qubits |
| Entangled state |  | Connected qubits, correlated outcomes |

Why This Analogy Works (and Its Limits)

What It Gets Right

- ✓ **Coherence** – The bubble is one object, just like a quantum state
- ✓ **Superposition** – The bubble is spread out, not localized
- ✓ **Probability** – Droplet landing follows bubble's "thickness" (Born rule)
- ✓ **Collapse** – Popping = measurement, instant and irreversible
- ✓ **Product states** – Separate bubbles = no entanglement
- ✓ **Entanglement** – Connected lobes = one joint state, two subsystems

What It Glosses Over (For Now)

- ⚠ Bubbles exist in 3D space – quantum states live in abstract Hilbert space
- ⚠ Bubbles have fixed shape – quantum states evolve continuously
- ⚠ Droplet analogy suggests particle-like outcome – **measurement gives a basis state, not a position**

A Glimpse Beyond (For the Curious)

This "Bubble Picture" Is Actually Real Mathematics

What we've drawn intuitively is closely related to **tensor network diagrams**



Both represent the same mathematical object – a tensor (generalized matrix).

Tensor networks are a powerful mathematical language used in:

- Quantum information theory
- Many-body physics
- Machine learning

In tensor networks:

- Bubbles = tensors (generalized matrices)
- Legs = indices (qubits)
- Connected bubbles = tensor contractions (interactions)

For now, enjoy the bubbles!

When you encounter tensor networks in later courses, you'll recognize the pictures immediately.

Multi-qubit gates

- **CNOT** (controlled-NOT): flips the target qubit if the control is $|1\rangle$.

Matrix (control = qubit 0, target = qubit 1):

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

- **Hadamard on two qubits**: creates superposition on both.

Example circuit to create a Bell state:

```
q0: —H—@—  
      |  
q1: —X—
```

Starting from $|00\rangle$:

1. H on q0: $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$
 2. CNOT: $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ – a Bell state.
-

Why Unitary? Schrödinger Equation

All quantum gates must be **unitary** ($U^\dagger U = I$). Why?

The time evolution of a closed quantum system is governed by the **Schrödinger equation**:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle,$$

where H is the Hamiltonian (Hermitian). The solution is

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle.$$

The operator $U = e^{-iHt/\hbar}$ is **unitary** because H is Hermitian.

Gates are discrete applications of such evolution operators.

Properties of unitary operators:

- They preserve the norm: $\langle \psi | \psi \rangle = \langle \psi | U^\dagger U | \psi \rangle = 1$.
- They are reversible: $U^{-1} = U^\dagger$.
- They map orthonormal bases to orthonormal bases.

This is why quantum computation is reversible (except measurement).

Summary and Next Lecture

Today we learned:

- Vector representation of qubits, basis states.
- The four postulates of quantum mechanics (state space, evolution, measurement, composition).
- Bloch sphere and rotation gates.
- Simple parameterized quantum circuits and training with PennyLane+Torch, including proper train/test split.
- Multi-qubit states, entanglement, and unitarity.

Next lecture (Week 3):

- Dirac notation in depth.
 - More quantum gates (Pauli, Hadamard, phase, CNOT, Toffoli).
 - Building quantum circuits.
 - Introduction to quantum algorithms (Deutsch-Jozsa).
-

Exercises

1. Bloch sphere coordinates

Write the states $|+\rangle$, $|-\rangle$, $|+i\rangle$, and $|-i\rangle$ in the form $\cos \frac{\theta}{2}|0\rangle + e^{i\phi} \sin \frac{\theta}{2}|1\rangle$. Verify their Bloch angles.

2. Rotation composition

Show that $R_y(\theta_1)R_y(\theta_2) = R_y(\theta_1 + \theta_2)$. What about R_x and R_z ?

3. Measurement probabilities

A qubit is in state $|\psi\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle$.

- What are the probabilities of measuring 0 and 1?
- After measuring 1, what is the new state?

4. Parameterized circuit

Modify the single-qubit predictor to use two trainable rotations ($R_y(\theta_1)$ and $R_z(\theta_2)$). Does it fit $\sin(x)$ better? Why or why not? (Hint: what functions can it represent now?)

5. Two-qubit state

Compute the state after applying H on qubit 0 and then CNOT (control=0, target=1) starting from $|01\rangle$. Is the resulting state entangled?

6. Unitarity check

Verify that the Pauli matrices are Hermitian and that $e^{-i\theta X/2}$ is unitary.

AI Tool Demo

This lecture's code examples were generated with the help of **DeepSeek**.

We used AI to:

- Suggest PennyLane syntax for parameterized circuits.
- Implement the train/test split with scikit-learn.
- Debug the training loop.
- Generate explanatory comments and exercises.

Remember: always understand what the code does before using it in your assignments.