Notes on Introduction to Quantum Computing

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1 Basic Concepts

1.1 Quantum bits (qubits)

Classical bits: $0, 1$

Quantum bit *qubit*: Superposition of 0 and 1:

A quantum state $|\psi\rangle$ is described as

$$|\psi\rangle := \alpha|0\rangle + \beta|1\rangle, \quad \alpha, \beta \in \mathbb{C} \tag{1}$$

where

$$|\alpha|^2 + |\beta|^2 = 1 \quad (normalization). \tag{2}$$

Mathematical description: $|\psi\rangle \in \mathbb{C}^2$ with

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \rightsquigarrow |\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Different from classical bits, cannot (in general) directly observe / measure a qubit (the amplitudes α and β). Instead: "*standard*" measurement will result in

- 0 with probability $|\alpha|^2$

- 1 with probability $|\beta|^2$

The measurement also changes the qubit (*wavefunction collapse*). If measuring 0, the qubit will be $|\psi\rangle = |0\rangle$ directly after the measurement, and likewise if measuring 1, the qubit will be $|\psi\rangle = |1\rangle$.

In practise: Can estimate the probabilities $|\alpha|^2$ and $|\beta|^2$ in experiments by repeating the same experiment many times (i.e via outcome statistics). These repetitions are called *trials* or *shots*.
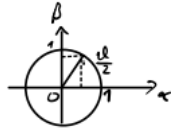

Figure 1: Circuit notation

A useful graphical deputation of a qubit is the Bloch sphere representation: If α and β happen to be real-valued, then can find angle $\vartheta \in \mathbb{R}$ such that

$$\alpha = \cos\frac{\vartheta}{2}, \quad \beta = \sin\frac{\vartheta}{2} \tag{3}$$

$$(\rightsquigarrow |\alpha|^2 + |\beta|^2 = \cos\frac{\vartheta}{2} + \sin\frac{\vartheta}{2}) = 1 \quad \checkmark$$
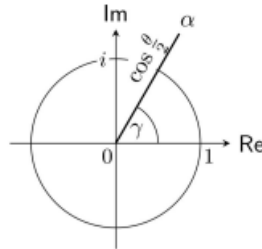

In general: represent

$$\alpha = e^{i\gamma} \cos\frac{\vartheta}{2}$$

$$\beta = e^{i(\varphi+\gamma)} \sin\frac{\vartheta}{2}$$

using so-called phase angles γ for α and $\varphi + \gamma$ for β.

Then:

$$|\psi\rangle = e^{i\psi} \cos\frac{\vartheta}{2} \cdot |0\rangle + \underbrace{e^{i(\varphi+\gamma)}}_{= e^{i\varphi} \cdot e^{i\gamma}} \sin\frac{\vartheta}{2} \cdot |1\rangle \tag{4}$$

$$= \underbrace{e^{i\gamma}}_{\text{can be ignored here}} \left(\cos\frac{\vartheta}{2} \cdot |0\rangle + e^{i\varphi} \cdot \sin\frac{\vartheta}{2} \cdot |1\rangle \right) \tag{5}$$

Thus $|\psi\rangle$ is characterized by two angles φ and γ; these specify the point defined as

$$\vec{r} = \begin{pmatrix} \cos\varphi \cdot \sin\vartheta \\ \sin\varphi \cdot \cos\vartheta \\ \cos\vartheta \end{pmatrix}$$
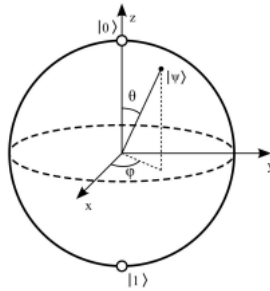
on the surface of a sphere:

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Figure 2: Bloch Sphere (Felix Bloch)

1.2 Single qubit gates

Principles of <u>time evolution</u>: The quantum state $|\psi\rangle$ at current time point t transitions to a new quantum state $|\psi'\rangle$ at a later time point $t' > t$.
Transition described by a complex unitary matrix U:

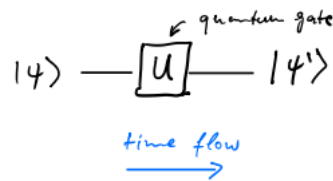$$|\psi'\rangle = U \cdot |\psi\rangle \tag{6}$$

Figure 3: Circuit notation

Notes:

- Circuit is read from left to right, but matrix times vector $(U|\psi\rangle)$ from right to left.

- U preserves normalization

Examples:

- Quantum analogue of the classical NOT gate $(0 \leftrightarrow 1)$ flip $|0\rangle \leftrightarrow |1\rangle$ leads to Pauli-X gate:

$$X \equiv \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{7}$$

Check: $X|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$ and $X|1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle$ ✓

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- Pauli-Y gate:
$$Y \equiv \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{8}$$

- Pauli-Z gate:
$$Z \equiv \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{9}$$

Z leaves $|0\rangle$ unchanged, but flips the sign of the coefficient of $|1\rangle$. Recall the Bloch Sphere representation:

$$|\psi\rangle = \cos\frac{\vartheta}{2} \cdot |0\rangle + e^{i\varphi} \sin\frac{\vartheta}{2} \cdot |1\rangle$$

Then

$$Z|\psi\rangle = \cos\frac{\vartheta}{2} \cdot |0\rangle \ - \ e^{i\varphi}\sin\frac{\vartheta}{2} \cdot |1\rangle$$

$$\overset{e^{i\pi}=-1}{=} \cos\frac{\vartheta}{2} \cdot |0\rangle + \underbrace{e^{i\pi}e^{i\varphi}}_{e^{i(\varphi+\pi)}}\sin\frac{\vartheta}{2} \cdot |1\rangle$$

⤳ new Bloch Sphere angles: $\vartheta' = \vartheta, \varphi = \varphi + \pi$ (rotating by $\pi = 180°$ around z-axis)

X, Y, Z gates are called <u>Pauli matrices</u>. The <u>Pauli vector</u> $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) = (X, Y, Z)$ is a vector of 2×2 matrices.

- Hadamard Gate:
$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\alpha\ |0\rangle \ + \ \beta\ |1\rangle \ ——\boxed{H}—— \ \alpha\ \frac{|0\rangle + |1\rangle}{\sqrt{2}} + \ \beta\ \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

Figure 4: Hadamard Gate

- Phase Gate:
$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

- T Gate:
$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

Note: $T^2 = S$ since $(e^{i\pi/4})^2 = e^{i\pi/2} = i$

Pauli matrices satisfy:

1. $\sigma_j^2 = I$ (identifity) for $j = 1, 2, 3$

2. $\sigma_j \cdot \sigma_k = -\sigma_k \sigma_j$ for all $j \neq k$

3. $[\sigma_j, \sigma_k] := \underbrace{\sigma_j \sigma_k - \sigma_k \sigma_j}_{\text{Commutator}} = 2i\sigma_l$ for (j, k, l) a cyclic permutation of (1,2,3).

General definition of $\underline{\text{matrix exponential}}$

$$exp(A) \equiv e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k, \quad A \in \mathbb{C}^{n \times n} \tag{10}$$

Special case: $A^2 = I, x \in \mathbb{R}$

$$e^{iAx} = \sum_{k=0}^{\infty} \frac{1}{(2k)!} (ix)^{2k} \underbrace{A^{2k}}_{(A^2)^k = I^k = I} + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (ix)^{2k+1} \underbrace{A^{2k+1}}_{(A^2)^k \cdot A = I^k \cdot A = A}$$

$$\underbrace{\phantom{\sum_{k=0}^{\infty} \frac{1}{(2k)!} (ix)^{2k} A^{2k}}}_{\text{even}} \quad \underbrace{\phantom{\sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (ix)^{2k+1} A^{2k+1}}}_{\text{odd}}$$

$$= \underbrace{\sum_{k=0}^{\infty} \frac{1}{(2k)!} (-1)^k x^{2k}}_{=\cos x} \cdot I + \underbrace{\sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (-1)^k x^{2k+1}}_{=i \sin x} \cdot A$$

$$= \cos x \cdot I + i \sin x A$$

(generalizes Euler's formula $e^{ix} = \cos x + i \sin x$)

This can be used to define the following $\underline{\text{rotation operators}}$ via the Pali matrices. Let $\vartheta \in \mathbb{R}$:

$$R_x(\vartheta) := e^{-i\vartheta X/2} = \cos\frac{\vartheta}{2} I - i \sin\frac{\vartheta}{2} X = \begin{pmatrix} \cos\frac{\vartheta}{2} & -i \sin\frac{\vartheta}{2} \\ -i \sin\frac{\vartheta}{2} & \cos\frac{\vartheta}{2} \end{pmatrix} \tag{11}$$

$$R_y(\vartheta) := e^{-i\vartheta Y/2} = \cos\frac{\vartheta}{2} I - i \sin\frac{\vartheta}{2} Y = \begin{pmatrix} \cos\frac{\vartheta}{2} & -\sin\frac{\vartheta}{2} \\ \sin\frac{\vartheta}{2} & \cos\frac{\vartheta}{2} \end{pmatrix} \tag{12}$$

$$R_z(\vartheta) := e^{-i\vartheta Z/2} = \cos\frac{\vartheta}{2} I - i \sin\frac{\vartheta}{2} Z = \begin{pmatrix} e^{-i\vartheta/2} & 0 \\ 0 & e^{i\vartheta/2} \end{pmatrix} \tag{13}$$

General case: Rotation about an axis $\vec{v} \in \mathbb{R}^3$ (normalized such that $\|\vec{v}\|) = \sqrt{v_1^2 + v_2^2 + v_3^3} = 1$):
using the notation:

$$\langle \vec{v}|\vec{\sigma}\rangle = \vec{v} \cdot \vec{\sigma} = v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3 = \begin{pmatrix} v_3 & v_1 - iv_2 \\ v_1 + iv_2 & -v_3 \end{pmatrix} \qquad (14)$$

It holds that $(\vec{v} \cdot \vec{\sigma})^2 = I$.
We define the rotation operator around axis $\vec{v}$ as

$$R_v(\vartheta) := e^{-i\vartheta(\vec{v}\cdot\vec{\sigma})/2} = \cos\frac{\vartheta}{2}I - i\sin\frac{\vartheta}{2}(\vec{v}\cdot\vec{\sigma}) \qquad (15)$$

Note: R_x, R_y, R_z are special cases corresponding to $\vec{v} = (1,0,0)$, $\vec{v} = (0,1,0)$, and $\vec{v} = (0,0,1)$.

Can derive that the Bloch Sphere representaiton of $R_{\vec{v}}(\vartheta)$ is a "conventional" rotation (in three dimensions) by angle ϑ about axis $\vec{v}$.
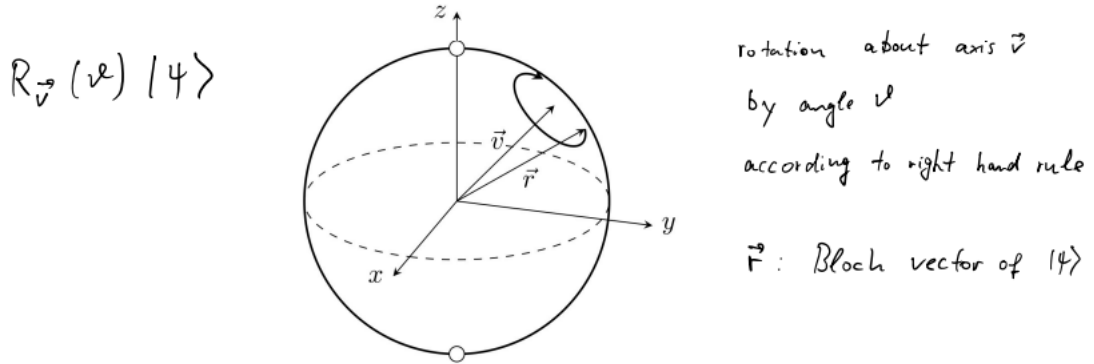

Figure 5: Circuit notation

Z-Y decomposition of an arbitrary 2×2 unitary matrix:
For any unitary matrix $U \in \mathbb{C}^{n \times n}$ there exist real numbers $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ such that

$$U = e^{i\alpha} \underbrace{\begin{pmatrix} e^{-i\beta/2} & 0 \\ 0 & e^{i\beta/2} \end{pmatrix}}_{R_z(\beta)} \cdot \underbrace{\begin{pmatrix} \cos\frac{\gamma}{2} & -\sin\frac{\gamma}{2} \\ \sin\frac{\gamma}{2} & \cos\frac{\gamma}{2} \end{pmatrix}}_{R_y(\gamma)} \cdot \underbrace{\begin{pmatrix} e^{-i\delta/2} & 0 \\ 0 & e^{i\delta/2} \end{pmatrix}}_{R_z(\delta)} \qquad (16)$$

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1.3 Multiple qubits

So far: Single qubits, superposition of basis states $|0\rangle$ and $|1\rangle$. For two qubits, this generalizes to $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

General two-qubit state:

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle \tag{17}$$

with amplitudes $\alpha_{ij} \in \mathbb{C}$ such that

$$|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1 \quad \text{(normalization)}. \tag{18}$$

Can identify the basis states with unit vectors:

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{19}$$

Thus:

$$|\psi\rangle = \begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix} \in \mathbb{C}^4 \tag{20}$$

What happens if we measure only one qubit of a two-qubit state? Say we measure the first qubit: Obtain result

$$\begin{array}{lll} 0 & \text{with probability} & |\alpha_{00}|^2 + |\alpha_{01}|^2 \\ 1 & \text{with probability} & |\alpha_{10}|^2 + |\alpha_{11}|^2 \end{array}$$

Wavefunction directly after measurement:

$$\text{if measured 0:} \quad |\psi'\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{01}|01\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{01}|^2}}$$

$$\text{if measured 1:} \quad |\psi'\rangle = \frac{\alpha_{10}|10\rangle + \alpha_{11}|11\rangle}{\sqrt{|\alpha_{10}|^2 + |\alpha_{11}|^2}}$$

Mathematical formalism for constructing two qubit states: Tensor product of vector space.
Can combine two (arbitrary) vector spaces V and W to form the tensor product $V \otimes W$.

The elements of $V \otimes W$ are linear combinations of "tensor products" $|v\rangle \otimes |w\rangle$ consisting of elements $|v\rangle \in V$ and $|w\rangle \in W$.

Example: Let $V = \mathbb{C}^2$ and $W = \mathbb{C}^2$ be the single qubit spaces with basis $\{|0\rangle, |1\rangle\}$, then

$$\underbrace{\frac{1}{2}|0\rangle \otimes |0\rangle}_{=|00\rangle} + \underbrace{\frac{5i}{7}|1\rangle \otimes |0\rangle}_{=|10\rangle} \in V \otimes W$$

Let $\{|i\rangle_v : i = 1, ..., m\}$ be a basis of of V, and let $\{|j\rangle_w : j = 1, ..., n\}$ be a basis of of W, then

$$\{|i\rangle_v \otimes |j\rangle_w : i = 1, ..., m, j = 1, ..., n\}$$

is a basis of $V \otimes W$. In particular, $dim(V \otimes W) = dim(V) \cdot dim(W)$.
Note: $|i\rangle_v \otimes |j\rangle_w$ is also written as $|ij\rangle$.

Basic properties of tensor product:

- $\forall |v\rangle \in V, |w\rangle \in W \wedge \alpha \in \mathbb{C}:$

$$\alpha(|v\rangle \otimes |w\rangle) = (\alpha|0\rangle) \otimes |w\rangle = |v\rangle \otimes (\alpha|w\rangle) \qquad (21)$$

- $\forall |v_1\rangle, |v_2\rangle \in V \wedge |w\rangle \in W:$

$$(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle \qquad (22)$$

- $\forall |v\rangle \in V \wedge |w_1\rangle, |w_2\rangle \in W:$

$$|v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle \qquad (23)$$

Vector notation using standard basis, e.g.

$$|v\rangle = v_1|0\rangle + v_2|1\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$

$$|w\rangle = w_1|0\rangle + w_2|1\rangle = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

$$|v\rangle \otimes |w\rangle = (v_1|0\rangle + v_2|1\rangle) \otimes (w_1|0\rangle + w_2|1\rangle)$$
$$= v_1 w_1|00\rangle + v_1 w_2|01\rangle + v_2 w_1|10\rangle + v_2 w_2|11\rangle$$

Thus:

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \otimes \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} v_1 w_1 \\ v_1 w_2 \\ v_2 w_1 \\ v_2 w_2 \end{pmatrix}$$

Note: Not every element of $V \otimes W$ can be written in the form $|v\rangle \otimes |w\rangle$, for example the Bell state

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

Assuming that V and W have an inner product $\langle \cdot | \cdot \rangle$, define inner product on $V \otimes W$ by

$$\langle \sum_j \alpha_j |v_j\rangle \otimes |w_j\rangle | \sum_k \beta_k |v_k\rangle \otimes |w_k\rangle \rangle := \sum_j \sum_k \alpha_j^* \beta_k \langle v_j | v_k \rangle \cdot \langle w_j | w_k \rangle \quad (24)$$

Generalization to n qubits: 2^n computational basis states