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

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

where

$$|\alpha|^2 + |\beta|^2 = 1$$
 (normalization). (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

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

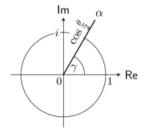
$$(\leadsto |\alpha|^2 + |\beta|^2 = \cos\frac{\vartheta}{2} + \sin\frac{\vartheta}{2}) = 1 \quad \checkmark$$
(3)



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:

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

$$\vec{r} = \begin{pmatrix} \cos \varphi \cdot \sin \vartheta \\ \sin \varphi \cdot \sin \vartheta \\ \cos \vartheta \end{pmatrix}$$

on the surface of a sphere:

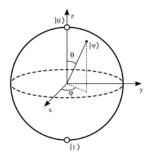


Figure 2: Bloch Sphere (Felix Bloch)

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:

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

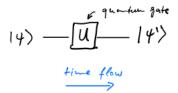


Figure 3: Circuit notation

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

• 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

$$\begin{split} Z|\psi\rangle &= \cos\frac{\vartheta}{2}\cdot|0\rangle - e^{i\varphi}\sin\frac{\vartheta}{2}\cdot|1\rangle \\ &\stackrel{e^{i\pi} \equiv -1}{=} \cos\frac{\vartheta}{2}\cdot|0\rangle + \underbrace{e^{i\pi}e^{i\varphi}}_{e^{i(\varphi+\pi)}}\sin\frac{\vartheta}{2}\cdot|1\rangle \end{split}$$

 \rightsquigarrow new Bloch Sphere angles: $\vartheta' = \vartheta, \varphi = \varphi + \pi$ (rotating by $\pi = 180^\circ$ 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:

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

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

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

General definition of matrix exponential

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

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

$$e^{iAx} = \underbrace{\sum_{k=0}^{\infty} \frac{1}{(2k)!} (ix)^{2k}}_{\text{even}} \underbrace{\underbrace{A^{2k}}_{(A^2)^k = I^k = I}}_{\text{even}} + \underbrace{\sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (ix)^{2k+1}}_{\text{odd}} \underbrace{\underbrace{A^{2k+1}}_{(A^2)^k \cdot A = I^k \cdot A = A}}_{\text{odd}}$$
$$= \underbrace{\sum_{k=0}^{\infty} \frac{1}{(2k)!} (-1)^k x^{2k} \cdot I}_{=\cos x} + \underbrace{\sum_{k=0}^{\infty} \frac{1}{(2k+1)!} (-1)^k x^{2k+1} \cdot A}_{=i\sin x}$$
$$= \cos x \cdot I + i\sin xA$$

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

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

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

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

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

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

It holds that $(\vec{v} \cdot \vec{\sigma})^2 = I$.

We define the rotation operator around axis \vec{v} as

$$R_{v}(\vartheta) := e^{-i\vartheta(\vec{v}\cdot\vec{\sigma})/2} = \cos\frac{\vartheta}{2}I - i\sin\frac{\vartheta}{2}(\vec{v}\cdot\vec{\sigma})$$
 (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 representation of $R_{\vec{v}}(\vartheta)$ is a "conventional" rotation (in three dimensions) by angle ϑ about axis \vec{v} .

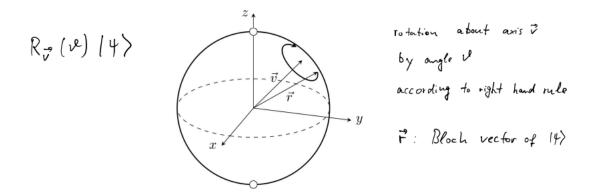


Figure 5: Circuit notation

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

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

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

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

0 with probability
$$|\alpha_{00}|^2 + |\alpha_{01}|^2$$

1 with probability $|\alpha_{10}|^2 + |\alpha_{11}|^2$

Wavefunction directly after measurement:

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

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

Mathematical formalism for constructing two qubit states: Tensor product of vector space.

Can combine two (arbitrary) vector spaces V and W to form the <u>tensor product</u> $V \otimes W$.

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 V, and let $\{|j\rangle_w: j=1,...,n\}$ be a basis 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:

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

$$\alpha(|v\rangle \otimes |w\rangle) = (\alpha|0\rangle) \otimes |w\rangle = |v\rangle \otimes (\alpha|w\rangle) \tag{21}$$

• $\forall |v_1\rangle, |v_2\rangle \in V \land |w\rangle \in W$:

$$(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle \tag{22}$$

• $\forall |v\rangle \in V \land |w_1\rangle, |w_2\rangle \in W$:

$$|v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle \tag{23}$$

Vector notation using standard basis, e.g.

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

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

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

$$= v_1w_1|00\rangle + v_1w_2|01\rangle + v_2w_1|10\rangle + v_2w_2|11\rangle$$

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

$$\{\underbrace{|0,...,0\rangle}_{\text{length }n}, |0,...,0,1\rangle,...|1,...,1\rangle\}$$

Thus: General n-qubit quantum state, also denoted as "quantum register", given by:

$$|\psi\rangle = \sum_{x_0=0}^{1} \sum_{x_1=0}^{2} \cdots \sum_{x_{n-1}}^{1} \alpha_{x_n-1,\dots,x_1,x_0} \cdot |x_{n-1},\dots,x_1x_0\rangle$$
 (25)

with $\alpha_x \in \mathbb{C}$ for all $x \in \{0, ..., 2^n - 1\}$, such that $\|\psi\|^2 = \sum_{x=0}^{2^n - 1} |\alpha_x|^2 = 1$ (normalization).

 \leadsto In general "hard" to simulate on classical computer (for large n) due to "curse of dimensionality".

Vector space as tensor products:
$$\underbrace{\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2}_{n \text{ times}} = (\mathbb{C}^2)^{\otimes n} = \mathbb{C}^{(2^n)}$$

1.4 Mutliple qubit gates

As for single qubits, an operation on multiple qubits is described by an unitary matrix U. For n qubits: $U \in \mathbb{C}^{2^n \times 2^n}$

Example: <u>controlled-NOT</u> gate (also CNOT): two qubits: <u>control</u> and target, target qubit gets flipped if <u>control</u> is 1:

$$|00\rangle \mapsto |00\rangle, \quad |01\rangle \mapsto |01\rangle, \quad |10\rangle \mapsto |11\rangle, \quad |11\rangle \mapsto |11\rangle$$

Can be expressed as

$$|a,b\rangle \mapsto |a,a\oplus b\rangle \quad \forall a,b \in \{0,1\}$$
 (26)

, where \oplus is the addition modulo 2.

Figure 6: CNOT circuit notation

Matrix representation:

$$U_{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$
 (27)

, with the Pauli-X matrix $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

Figure 7: Alternative CNOT circuit notation

Can generalize Pauli-X to any unitary operator U acting on target qubit \rightsquigarrow controlled-U gate:

Figure 8: Controlled-U gate



Figure 9: Example: Controlled-Z gate

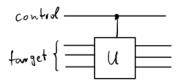


Figure 10: Controlled-U for multiple target qubits

Note: Single qubit and CNOT gates are <u>universal</u>: They can be used to implement an arbitrary unitray operation on n qubits (Quantum analogue of university of classical NAND gate). Proof in Nielsen and Chuang section 4.5.

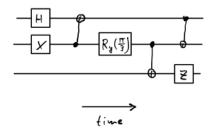
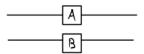


Figure 11: Example of a circuit lousisting only of single qubit gates and ${
m CNOTs}$

1.4.1 Matrix Kronecker Products

Matrix representation of single qubit gates acting in parallel:



Operation on basis states: $a, b \in \{0, 1\}$:

$$|a,b\rangle \mapsto (A|a\rangle) \otimes (B|b\rangle)$$
 (28)

Example:
$$A = I$$
 (identity), $B = Y$

$$|00\rangle \mapsto |0\rangle \otimes (Y|0\rangle) = i|01\rangle$$

$$|01\rangle \mapsto |0\rangle \otimes (Y|1\rangle) = -i|00\rangle$$

$$|10\rangle \mapsto |1\rangle \otimes (Y|0\rangle) = i|11\rangle$$

$$|11\rangle \mapsto |1\rangle \otimes (Y|1\rangle) = -i|10\rangle$$

Matrix representation:

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

Figure 12: Circuit notation

General formula: <u>Kronecker product</u> (matrix representation of tensor products of operators)

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{pmatrix} \in \mathbb{C}^{mp \times nq}$$
 (29)

for all $A \in \mathbb{C}^{m \times n}$ and $B \in \mathbb{C}^{p \times q}$.

Another example:
$$\frac{y}{i} = \begin{pmatrix} 0.I & -i.I \\ i & 0.I \end{pmatrix} = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}$$

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Figure 13: Generalization to arbitrary number of tensor factors possible

Basic properties:

1. $(A \otimes B)^* = A^* \otimes B^*$ (elementwise complex conjugation)

2.
$$(A \otimes B)^T = A^T \otimes B^T$$
 (transposition)

- 3. $(A \otimes B)^{\dagger} = A^{\dagger} \otimes B^{\dagger}$
- 4. $(A \otimes B) \otimes C = A \otimes (B \otimes C)$ (associative property)
- 5. $(A \otimes B) \cdot (C \otimes D) = (A \cdot C) \otimes (B \cdot D)$ (for matrix of compatible dimensions)

- 6. Kronecker product of Hermitian matrices is Hermitian.
- 7. Kronecker product of unitary matrices is unitary (follows from 3. and 5.)

2 Quantum measurement