### Methods in quantum computing

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- Problem set 0 (Optional):
  - one more week
  - Question 1 does NOT have a typo
- Problem set 1:
  - Bonus question involves regular addition, not mod 2
- atb=c
- you can use CNOTS, Toff and any single qubit gates
- · it just needs to work
- submit through email/Canvas/Teams
- you can update your solutions before the deadline if you want to

- 1. More circuits
- 2. Linear algebra
- 3. Quantum states
- 4. Quantum operations
- 5. No-cloning theorem (if we have time)
- 6. Measurement (if we have time)

#### Pauli Z and X

$$z | 0 \rangle = | 0 \rangle$$

$$z | 1 \rangle = -11 \rangle$$

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

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

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

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

$$x = 1 \wedge 1 | 1 \times 1 |$$

$$x = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = | 0 \times 0 | + | 1 \times 1 |$$

$$x = \int x = \int x = 1 | 0 \times 0 | + | 1 \times 1 |$$

$$x = \int x = \int x = 1 | 0 \times 0 | + | 1 \times 1 |$$

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#### Exercise

Compute XZX and ZXZ

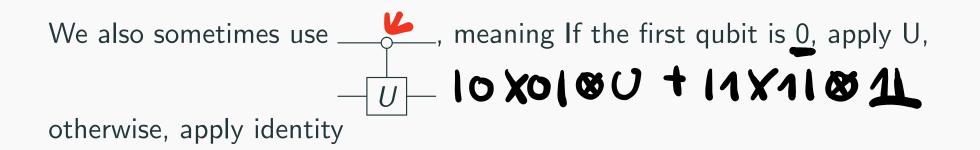
#### **Controlled** gates

otherwise, apply identity

If the first qubit is 1, apply U,

11×1100 + 10×0101

# $CNOT = |OXO| \otimes (1 + |1X1| \otimes X) = |OXO| \otimes (|OXO| + |1X1|) + |1X1| \otimes (|OX1| + |1X0|)$



#### Linear algebra

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A d-dimensional Hilbert space  $\mathcal{H}$  is a vector space equipped with an inner product. Let  $\{e_i\}_{i=0}^{d-1}$  be the computational basis, where  $e_i$  is a column vector of zeros except a '1' at the (i + 1)-th entry. Any vector  $\mathbf{v} \in \mathcal{H}$  can be decomposed into basis vectors  $e_i$  as  $\mathbf{v} = \sum_{i=0}^{d-1} v_i e_i$ , linear comb of basis vectors (1)

for some complex number  $v_i \in \mathbb{C}$ . The inner product (or dot product) '·'

of two vectors  $\boldsymbol{u}$  and  $\boldsymbol{v}$  in the same basis in  $\mathcal H$  is defined as

$$\boldsymbol{u} \cdot \boldsymbol{v} = \boldsymbol{u}^{\dagger} \boldsymbol{v} = \sum_{i=0}^{d-1} u_i^* v_i, \quad \text{this is how}$$
  
it's computed

where † denotes transpose and conjugate.

#### **Dirac notation**

basis vector Denote  $|i\rangle \equiv e_i$  and write  $\mathbf{v}$  as  $|\mathbf{v}\rangle$ : d-1 $|v\rangle = \sum v_i |i\rangle.$ (3)decat bra < 1ket 1 >The inner product braket  $\mathbf{A}^{\dagger} \mathbf{T} \cdot \langle u | v \rangle = \sum_{i,j} u_i^* v_j \langle i | j \rangle = \sum_i u_i^* v_i$ (4)where  $\langle u | \equiv |u\rangle^{\dagger}$  is now a row vector and  $\langle i | j \rangle = \delta_{i,j}$ i=j -> <i |j>=1 i=j -> <i |j>=0 Kronecker delta  $\begin{cases} 1 & if i=j \\ 0 & i\neq j \end{cases}$ 

#### **Vector space basis**

for each ii, iii = 1if  $i \neq i$ ,  $i \neq i$ , Linear maps

#### $L: U \rightarrow V$

Example: Matrix multiplication

Given an linear operator L, there is an equivalent matrix representation [ $L_{i,k}$ ] in the basis spanned by { $|i\rangle\langle k|$ }:

$$L = \sum_{i,k=0}^{d-1} L_{i,k} |i\rangle \langle k|, \quad \text{Coolicy}. \quad (5)$$

where  $L_{i,k} = \langle i | L | k \rangle$ .

An linear operator  $H \in \mathcal{L}(\mathcal{H})$  is called <u>Hermitian</u> iff  $H^{\dagger} = H$ . For a Hermitian matrix H, the spectral theorem states that there exists an

orthonormal basis  $\{|\nu_i\rangle\}$  and real numbers  $\{\lambda_i\} \in \mathbb{R}$  so that  $H = \sum \lambda_i |\nu_i\rangle \langle \nu_i |.$   $M = \begin{pmatrix} A_A & O \\ A_A & A_A \end{pmatrix}$  (6)

i  
Equivalently, 
$$\{\lambda_i\}$$
 and  $\{|\nu_i\rangle\}$  are known as eigenvalues and eigenvectors  
of *H*, respectively.

Verify that Pauli X is a Hermitian operator and compute its eigenvalues and eigenvectors.

in

Given two vectors  $|u\rangle \in \mathcal{H}_A$  and  $|v\rangle \in \mathcal{H}_B$ , the tensor product ' $\otimes$ ' of them is

$$\begin{split} \mathbf{I}_{A,V} = |u\rangle \otimes |v\rangle &= \sum_{i=0}^{d_{A}-1} \sum_{j=0}^{d_{B}-1} u_{i}v_{j}|i\rangle \otimes |j\rangle, \end{split} \tag{7} \\ \text{normalized mut.orthogonal} \\ \text{a vector of } d_{A}d_{B} \text{-dimension. If } \{|i\rangle_{A}\} \text{ and } \{|j\rangle_{B}\} \text{ are orthonormal bases} \\ \text{in } \mathcal{H}_{A} \text{ and } \mathcal{H}_{B}, \text{ respectively, then } \{|i\rangle_{A} \otimes |j\rangle_{B}\}, i \in \{0, \cdots, d_{A}-1\} \text{ and} \\ j \in \{0, \cdots, d_{B}-1\}, \text{ forms an orthonormal basis in } \mathcal{H}_{A} \otimes \mathcal{H}_{B}. \text{ The inner} \\ \text{product on the space } \mathcal{H}_{A} \otimes \mathcal{H}_{B} \text{ is defined by} \end{split}$$

$$(\langle u_1|_A \otimes \langle u_2|_B) (|v_1\rangle_A \otimes |v_1\rangle_B) = \langle u_1|v_1\rangle \langle u_2|v_2\rangle.$$
(8)  
$$|01\rangle = |0\rangle \otimes |1\rangle \quad \langle 01|11\rangle = \langle 01|1\rangle \cdot \langle 1|1\rangle = \langle 01|1\rangle \cdot \langle 1|1\rangle = \langle 01|1\rangle = \langle 01|1\rangle + \langle 01|1\rangle = \langle 0$$

Linear operators in 
$$\mathcal{L}(\mathcal{H})$$
:  

$$\mathcal{L} \otimes M = \begin{pmatrix} \sum_{i,j=0}^{d_A-1} L_{i,j} |i\rangle \langle j| \\ \sum_{k,\ell=0}^{d_B-1} M_{k,\ell} |k\rangle \langle \ell|, \end{pmatrix}$$

$$= \sum_{i,j=0}^{d_A-1} \sum_{k,\ell=0}^{d_B-1} L_{i,j} M_{k,\ell} \overline{i\rangle \langle j| \otimes |k\rangle \langle \ell|}.$$
(9)

Trace

$$A = \left( \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \right) \quad Tr(A) = \sum_{i} A_{i,i}$$

The trace maps is defined as

$$\operatorname{Tr}|j\rangle\langle k| = \langle k|j\rangle = \delta_{k,j}.$$
(10)

From linearity, the trace of an operator L is

$$\operatorname{Tr} L = \underbrace{\sum_{i=0}^{d-1} \langle i|L|i \rangle}_{j} = \sum_{j} L_{j,j}.$$
 (11)

Tr maps operator to a scalar

#### Exercise

**1** • Cyclic property: Show that Tr LM = Tr ML. **2** • Show that Tr A is independent of the basis of A. ドン -> リバン  $T_r(LM) = \frac{\sum_{i} \sum_{j} \sum_{j$  $= \sum_{i} \langle i | L_{i} \rangle \langle j | M | i \rangle = \sum_{i} \langle j | M \times i | i \times L_{i} \rangle$ Scalars = $\Sigma_{j}$  (jIML|j) = Tr(ML) 2. Tr(A)= $\Sigma_{j}$  (i) Ali) (i) ->Uli)  $Tr(A) = \Sigma_{i} \langle i | u^{\dagger} A U | i \rangle = \Sigma_{i} \langle i | A \cup U^{\dagger} | i \rangle = \Sigma_{i} \langle i | A | i \rangle$ = Tr(A)

A generalization of a trace. Partial trace maps an operator to a lower-dimensional operator. Formally, partial trace  $\operatorname{Tr}_A : \mathcal{L}(\mathcal{H}_{AB}) \to \mathcal{L}(\mathcal{H}_B)$  is defined by  $\mathsf{Tr}_{A}\left(|i\rangle\langle j|_{A}\otimes|k\rangle\langle \ell|_{B}\right)=\langle j|i\rangle|k\rangle\langle \ell|_{B}=\delta_{i,j}|k\rangle\langle \ell|_{B}.$ (12)lixila 4 LIKZ Tra For a composite system on the space  $\mathcal{H}_A \otimes \mathcal{H}_B$ ,  $\operatorname{Tr}_A$  gives trace only over the subsystem on  $\mathcal{H}_A$  and remains subsystem  $\mathcal{H}_A$  intact. We often say that we "trace-over A".

# < 1 >

Use the ket notation  $|\cdot\rangle$  to denote a column vector of length one, e.g.,

$$|\psi\rangle := \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \tag{13}$$

and use the bra notation  $\langle \cdot |$  to denote the hermitian conjugate of  $| \cdot \rangle$ :

$$\langle \psi | := \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix}. \tag{14}$$

An alternative representation of a quantum state is the density matrix. For pure states:

$$\sigma_{\psi} = |\psi\rangle \langle \psi| \tag{15}$$
**Projector on 14>**

Given  $|\psi\rangle_A \in \mathcal{H}_A$  and  $|\phi\rangle_B \in \mathcal{H}_B$ , the joint quantum state is  $|\varphi\rangle_{AB} \equiv |\psi\rangle_A \otimes |\phi\rangle_B \in \mathcal{H} \equiv \mathcal{H}_A \otimes \mathcal{H}_B.$ 

If one of the subsystems, say  $\mathcal{H}_A$ , is lost from  $|\varphi\rangle_{AB}$ , the residue quantum state can be expressed as

$$\sigma_B = \operatorname{Tr}_A |\varphi\rangle\langle\varphi|. \tag{16}$$

#### 142

 $\sigma_B$  isn't always a pure state but a mixture of states  $\sigma_B := \sum_i p_i |\psi_i\rangle \langle \psi_i |$ where  $|\psi_i\rangle$  are orthogonal pure states on the subsystem B. There are three necessary and sufficient criteria that a matrix corresponds to a valid description to a quantum state. Show that

$$\mathbf{\hat{S}} \bullet := \sum_{i} p_{i} |\psi_{i}\rangle \langle \psi_{i}|, \quad \mathbf{\hat{S}} = \begin{pmatrix} \mathbf{P} \bullet \mathbf{P}_{1} & \mathbf{O} \\ \mathbf{O} & \mathbf{P}_{2} \\ \mathbf{O} & \mathbf{P}_{2} \end{pmatrix}$$
(17)

where  $\sum_{i} \rho_{i} = 1$  satisfies all three of them  $\neg all Pi \quad Satisfy \quad O \leq P_{i} \leq 1 \quad \mu \text{ real}$   $1. \rho \text{ is Hermitian } \uparrow \uparrow = \Sigma_{i} P_{i}^{*} (|\Psi_{i} X \Psi_{i}|)^{+} = \Sigma_{i} P_{i} \quad |\Psi_{i} X \Psi_{i}|$   $2. \rho \text{ is positive semi-definite } ^{2}$  $3. \text{Tr}[\rho] = 1.$ 

have at 174

<sup>&</sup>lt;sup>1</sup>A hermitian matrix A satisfies  $A^{\dagger} = A$ .

<sup>&</sup>lt;sup>2</sup>Eigenvalues of a positive semi-definitive matrix are real and equal to 0 or positive.

Not pure states:

- outcome of a random preparation
- part of a larger entangled state

An ensemble of pure states  $\mathcal{E} : \{p_i, |\psi_i\rangle\}$  can be denoted by a density operator

$$\sigma := \sum_{i} p_{i} |\psi_{i}\rangle \langle \psi_{i}|, \qquad (18)$$

where  $|\psi_i\rangle$  are individual states that could be prepared and  $p_i$  are the corresponding probabilities. We refer to objects  $\sigma$  as **density matrices**.

71: 10007 
$$\frac{1}{6}$$
 (300×00)  
2: 10017 6  
3: 10107  
4: 10117  
5: 11017  
6: 11017

If  $\rho$  is pure, it can be written as a projector on the corresponding pure state  $|\psi\rangle$ 

$$\sigma_{\psi} = |\psi\rangle\langle\psi|. \tag{19}$$

Projectors have the property that  $(|\psi\rangle\langle\psi|)^2 = |\psi\rangle\langle\psi|$ 

$$\frac{1}{1} = \frac{1}{1} = \frac{1}{1} + \frac{1}{1} = \frac{1}{1} + \frac{1}{1} = \frac{1}{1} + \frac{1}{1} + \frac{1}{1} = \frac{1}{1} + \frac{1}$$

Let  $|\Phi\rangle_{AB} = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B)$ . Compute  $\text{Tr}_A(|\Phi\rangle\langle\Phi|_{AB})$  and  $\text{Tr}_B(|\Phi\rangle\langle\Phi|_{AB})$ . Discuss whether the result could be a pure state (no need to prove it).

Suppose that the person, say Alice, who prepares this ensemble can keep track of 'which state' she prepared. In other words, she has the additional classical label  $|x\rangle\langle x|$  attached to the state  $\sigma_x \in \mathcal{D}(\mathcal{H}_B)$ , where  $\{|x\rangle\}$  forms an orthonormal basis of  $\mathcal{H}_X$ . Such a hybrid classical-quantum system can be described as

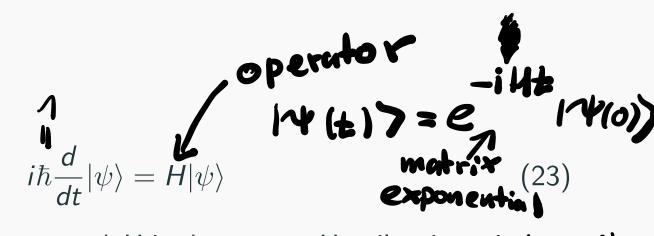
$$\sigma_{XB} = \sum_{x \in \mathcal{X}} p_x |x\rangle \langle x| \otimes |\psi_x\rangle \langle \psi_x|.$$
(20)  
purification - adding another  
system to represent a density operator  
is a part of a pure state

$$|\psi\rangle \to U |\psi\rangle.$$
 (21)

For a general quantum state described by a density matrix (21) takes form

$$\rho \rightarrow U\rho U^{\dagger} = \sum_{i} U |\psi_{i}\rangle \langle\psi_{i}| U^{\dagger}.$$
(22)
  
conjugat<sup>i</sup> on
  
initary sandwich

#### Schrödinger equation



where  $\hbar$  is the Planck constant and H is the system Hamiltonian. C hermitian Eigenvalues of Hamiltonian define the allowed energies of a system.

Physicists and chemists really care about this!!

#### Exercise

Define purity of a quantum state as  $Tr[\rho^2]$ . Show that unitary operations preserve purity, i.e. a pure state never gets mapped onto a mixed state and vice versa.

# If q is pure then $g^2 = \int (projector)$ so $Tr(g^2) = Tr(l) = 1$

Channels are the most general operation of quantum states. They must be always map quantum states onto quantum states, even if if we apply the channel only on a subset of qubits. Any such channel can be written as

$$\Phi(\sigma) = \sum_{i} B_{i} \sigma B_{i}^{\dagger} \text{ where } P_{i} = 1.$$
(24)
Kraus decomposition
$$Z_{i} B_{i}^{\dagger} B_{i}^{\dagger} = 1.$$

# **Theorem (No-Cloning theorem)** There is no unitary operation $U_{copy}$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ such that for all $\mathcal{H}_A \in \mathcal{H}_A$ and $|0\rangle_B \in \mathcal{H}_B$ $\mathcal{H}_{copy}(|\phi\rangle_A \otimes |0\rangle_B) = e^{if(\phi)} |\phi\rangle_A \otimes |\phi\rangle_B$ (25)

for some number  $f(\phi)$  that depends on the initial state  $|\phi\rangle$ .

Prove the no-cloning theorem by contradiction. on 4 a Assuming  $U_{copy}$  exists, take two states  $|\phi_{\perp}\rangle$  and  $|\psi\rangle$ . Now apply  $U_{\rm copy}$  on both of them and compute the resulting inner product  $(\langle \phi |_A \otimes \langle 0 |_B) U^{\dagger}_{\text{copy}} U_{\text{copy}} (|\psi \rangle_A \otimes |0 \rangle_B).$ E b Explain how (a) leads to a contradiction. EN() 107 E 107 or 117  $- \frac{1000}{100} \rightarrow \frac{100}{100}$ 

Obtain classical information from a quantum state. It can destroy the superposition property of a quantum state.

Observe this qubit in state  $|0\rangle$  with probability  $|\alpha|^2$  and in state  $|1\rangle$  with probability  $|\beta|^2$ . Furthermore, after the measurement, the qubit state  $|b\rangle$  will disappear and collapse to the observed state  $|0\rangle$  or  $|1\rangle$ .



A collection of  $\Upsilon := \{M_i\}$ , where each measurement operator  $M_i \in \mathcal{L}(\mathcal{H})$  satisfies

$$\sum_{i} M_{i} = I \tag{26}$$

and each  $M_i$  is positive semi-definite operator. We call this measurements positive operator-valued measure (POVM). The probability of obtaining an outcome *i* on a quantum state  $\rho$  is

$$p_i := \operatorname{Tr}(M_i \rho). \tag{27}$$

The state after measurement will be altered as

$$\rho_i := \frac{M_i \rho}{p_i}.$$

Each  $M_i$  is a projector

$$p_j := \operatorname{Tr}\left(P_j |\phi\rangle\langle\phi|
ight)$$

and the resulting state

$$\frac{P_j |\phi\rangle}{\sqrt{p_j}}$$