Generalized Quantum States

via Mixed States and Density Operators

Fernando Granha Jeronimo

(Updated: 04/12/25)

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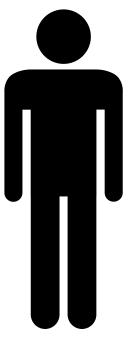
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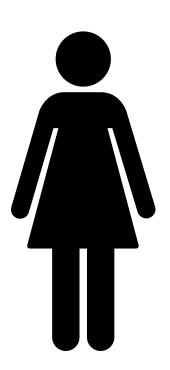
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Is this kind of description sufficient?

Scenario 1

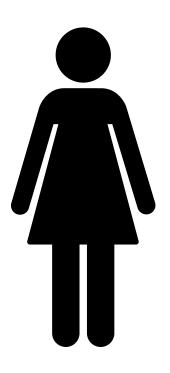






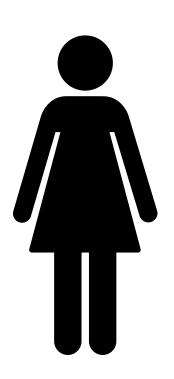


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$$|\mathbf{EPR}\rangle = \frac{1}{\sqrt{2}}|0\rangle^A|0\rangle^B + \frac{1}{\sqrt{2}}|1\rangle^A|1\rangle^B \neq |\psi_A\rangle \otimes |\psi_B\rangle$$

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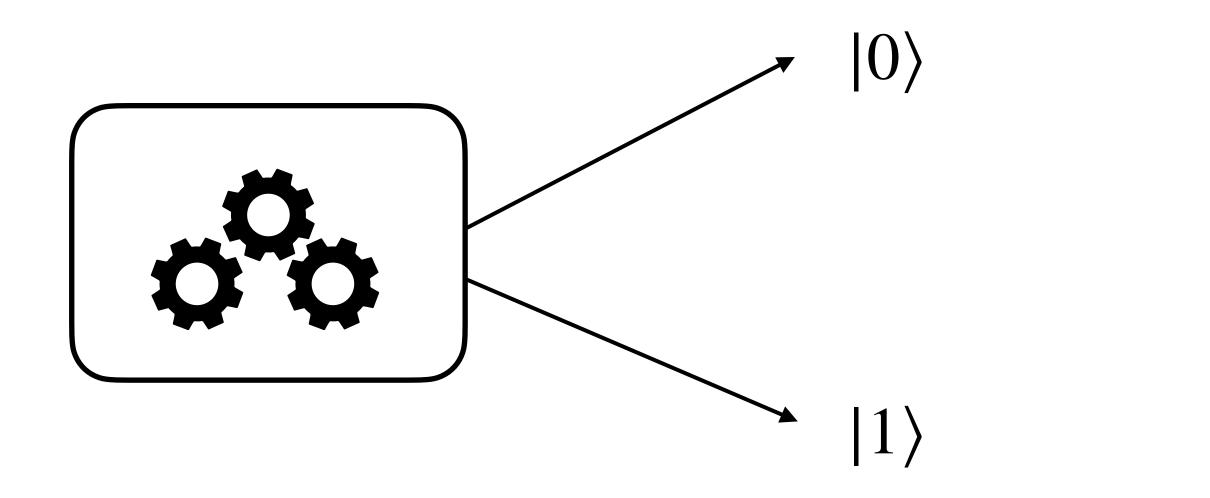
It is not a pure state!

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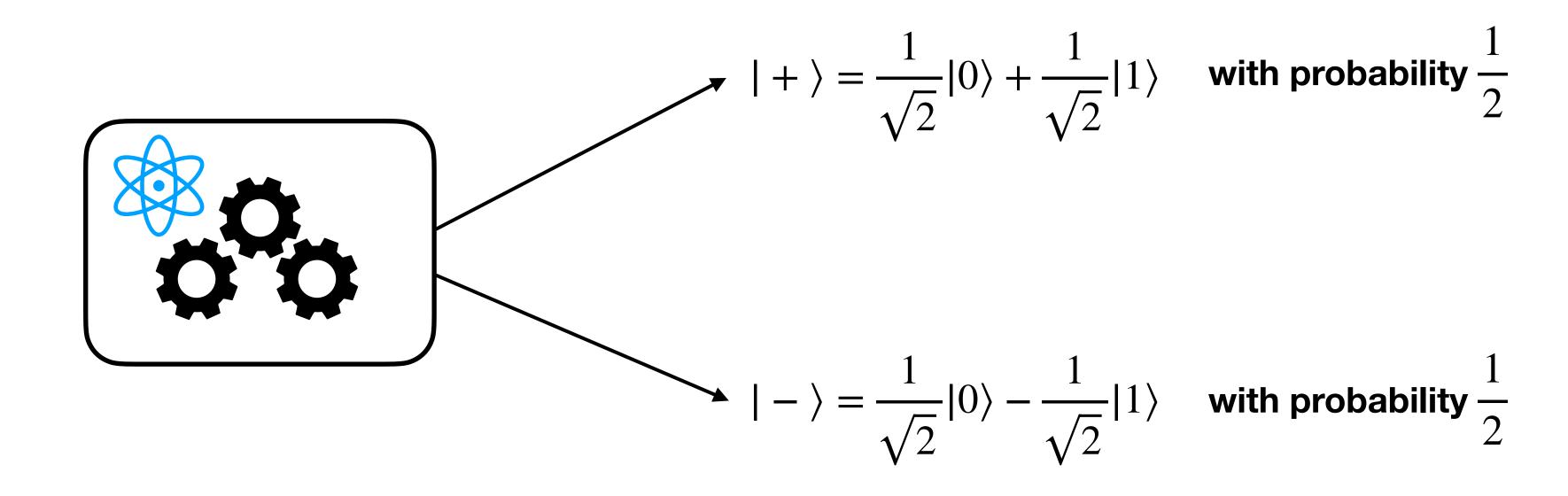
Suppose a Classical Machine Produces States



with probability $\frac{1}{2}$

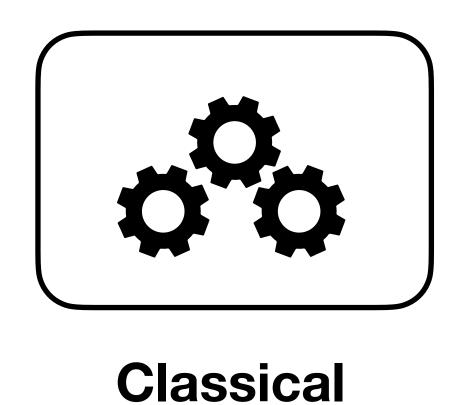
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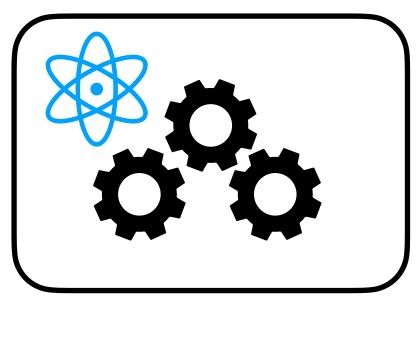
Suppose a Quantum Machine Produces States



How can we describe the output quantum state?

How different are the outputs of these machines?





Quantum

We need a more general formalism to describe quantum states!

The Ensemble Formalism

 $[m] = \{1, 2, ..., m\}$

Given

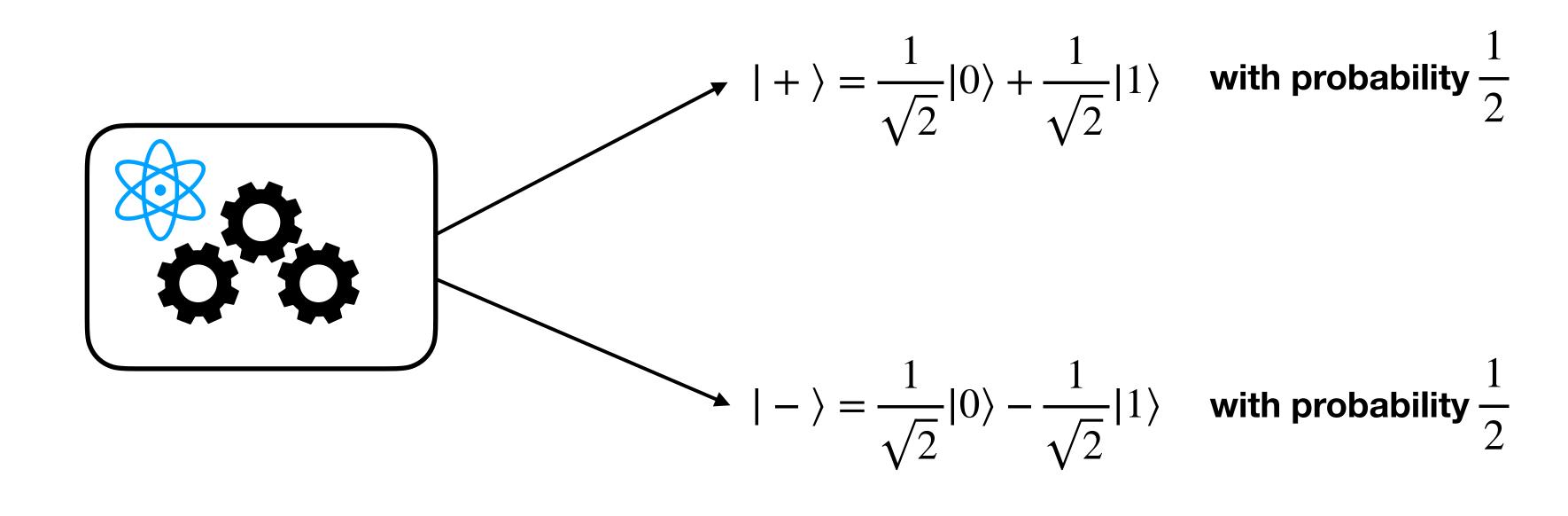
(1) $\{p_i\}_{i\in[m]}$ probability distribution $\left(\sum_{i=1}^m p_i = 1, p_i \ge 0 \,\forall i \in [m]\right)$ and

(2) $\{|\psi_i\rangle\in\mathbb{C}^d\}_{i\in[m]}$ pure quantum states,

we define the ensembe of quantum states:

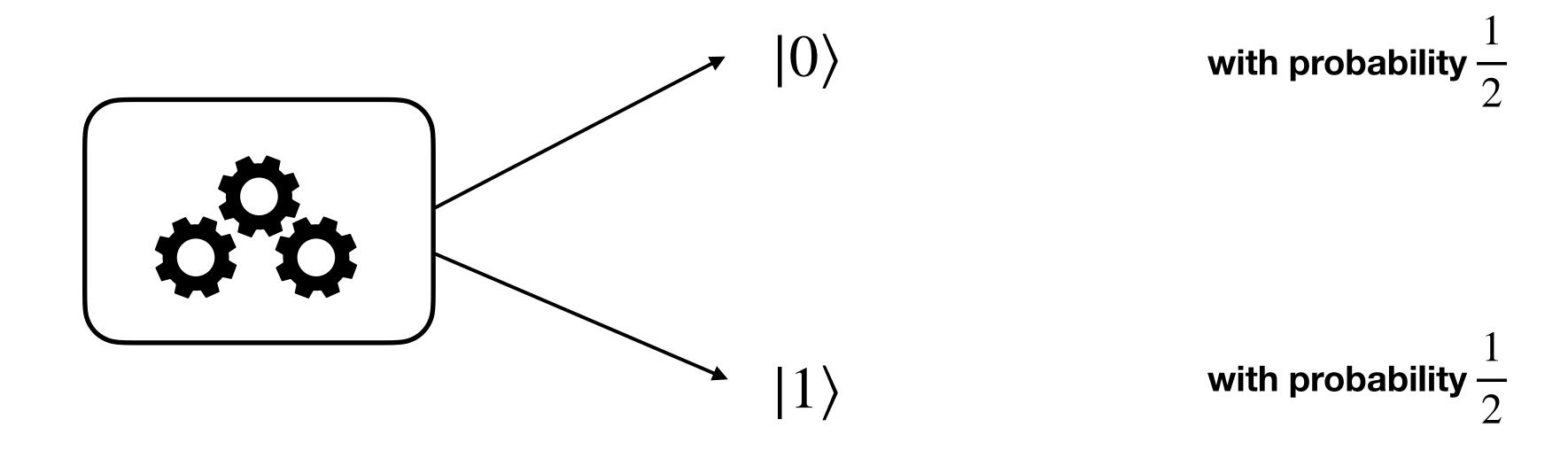
$$\left\{ \left(p_i, |\psi_i \rangle \right) \right\}_{i \in [m]}$$

Exemple of Ensembles



$$\left\{ \left(\frac{1}{2}, |+\rangle \right), \left(\frac{1}{2}, |-\rangle \right) \right\}$$

Exemple of Ensembles



$$\left\{ \left(\frac{1}{2}, |0\rangle\right), \left(\frac{1}{2}, |1\rangle\right) \right\}$$

Exemple of Ensembles

 $|\psi\rangle\in\mathbb{C}^d$ (a pure quantum state)

$$\{(1,|\psi\rangle)\}$$

Density Operator Formalism

A quantum state is a matrix $\rho \in \mathbb{C}^{d \times d}$ satisfying

- (1) $Tr(\rho) = 1$
- (2) $\rho \geq 0$ positive semi-definite (PSD), i.e., $\rho = \rho^{\dagger}$ and $\langle \phi | \rho | \phi \rangle \geq 0, \forall | \phi \rangle \in \mathbb{C}^d$

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Answer:

$$\rho = \sum_{i=1}^{m} p_i |\psi_i\rangle\langle\psi_i|$$

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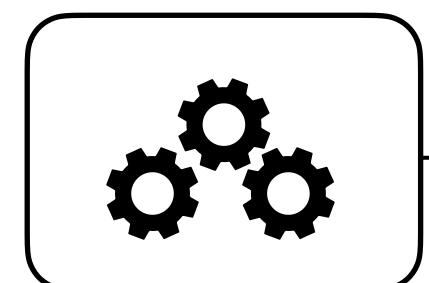
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(3)
$$\langle \phi | \rho | \phi \rangle = \sum_{i=1}^{m} p_i \langle \phi | \psi_i \rangle \langle \psi_i | \phi \rangle = \sum_{i=1}^{m} p_i |\langle \phi | \psi_i \rangle|^2 \ge 0, \forall |\phi \rangle \in \mathbb{C}^d$$

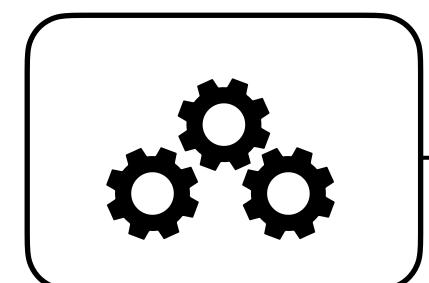
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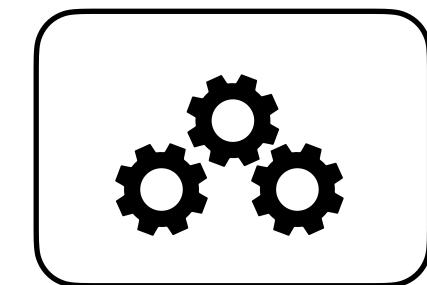
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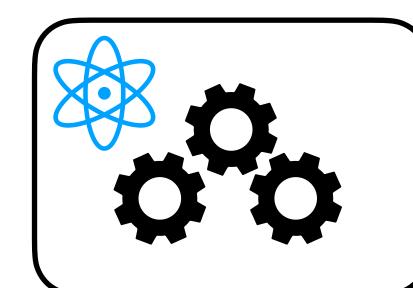
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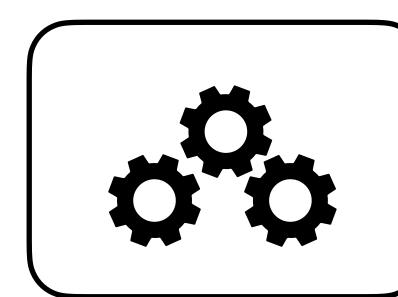
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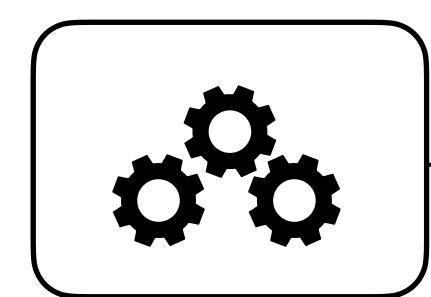
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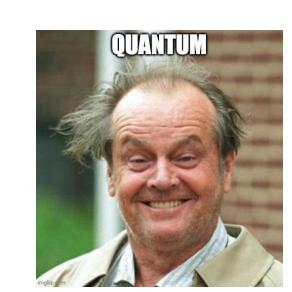
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A More General Principle

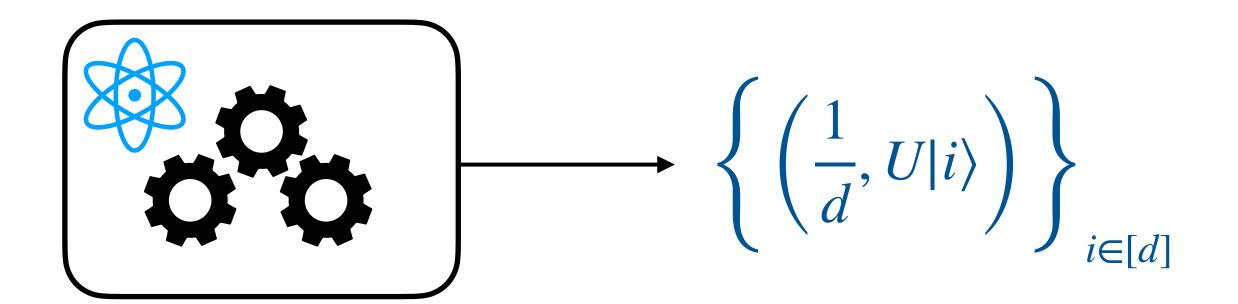
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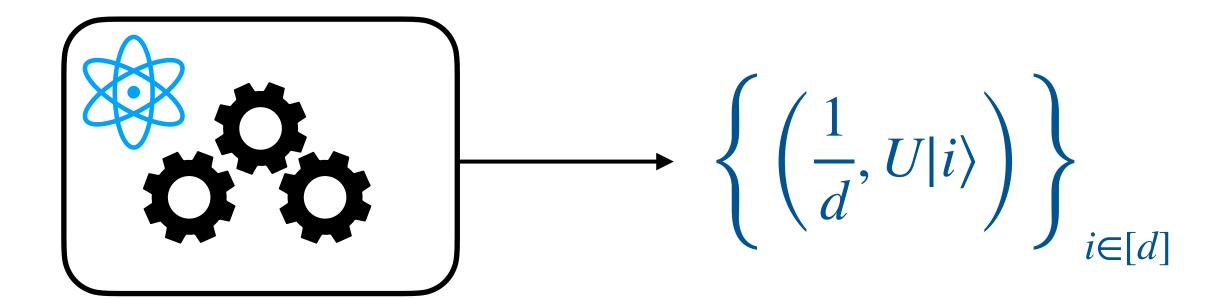
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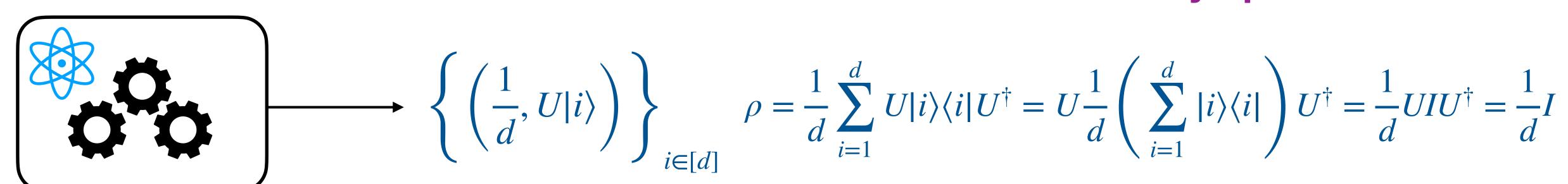
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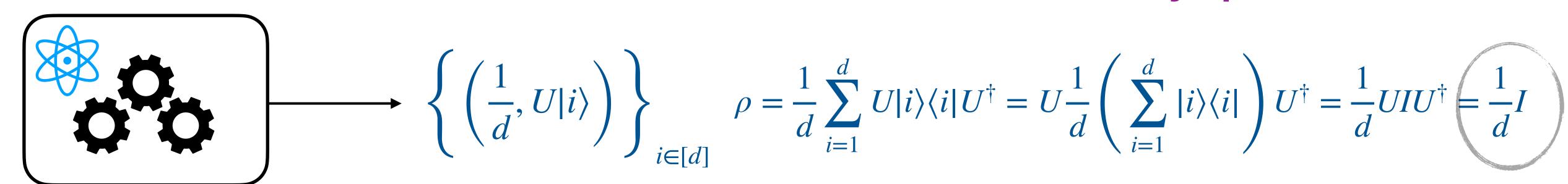
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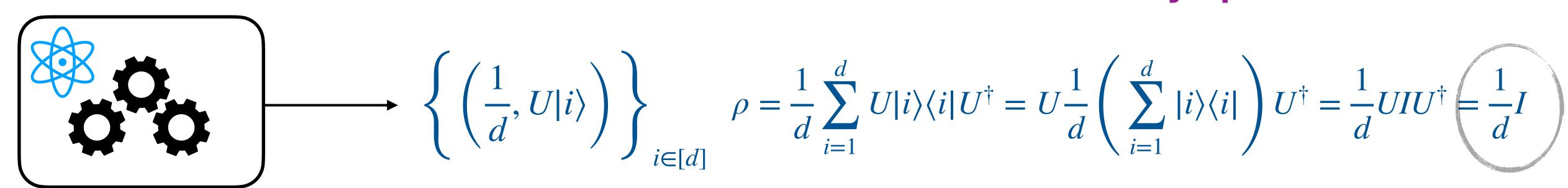


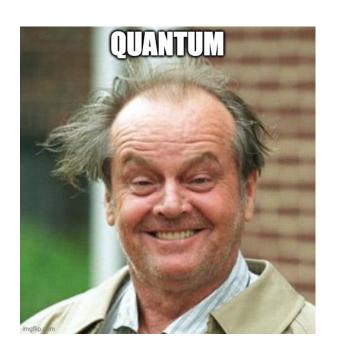
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For this, we will invoke the Spectral Theorem from Linear Algebra!

Refresher on the Spectral Theorem

[Spectral Theorem]

Given a normal matrix $A \in \mathbb{C}^{d \times d}$ (i.e., $AA^{\dagger} = A^{\dagger}A$), there exist

- (1) Orthonomal basis of eigenvectors $\{|\psi_i\rangle\}_{i\in[d]}$, and
- (2) Correspoding Eigenvalues $\{\lambda_i\}_{i\in[d]}$ (i.e., $A|\psi_i\rangle=\lambda_i|\psi_i\rangle$), such that

$$A = \sum_{i=1}^{d} \lambda_i |\psi_i\rangle \langle \psi_i|$$

Refresher on the Spectral Theorem

In particular, this theorem holds for Hermitian and unitary matrices

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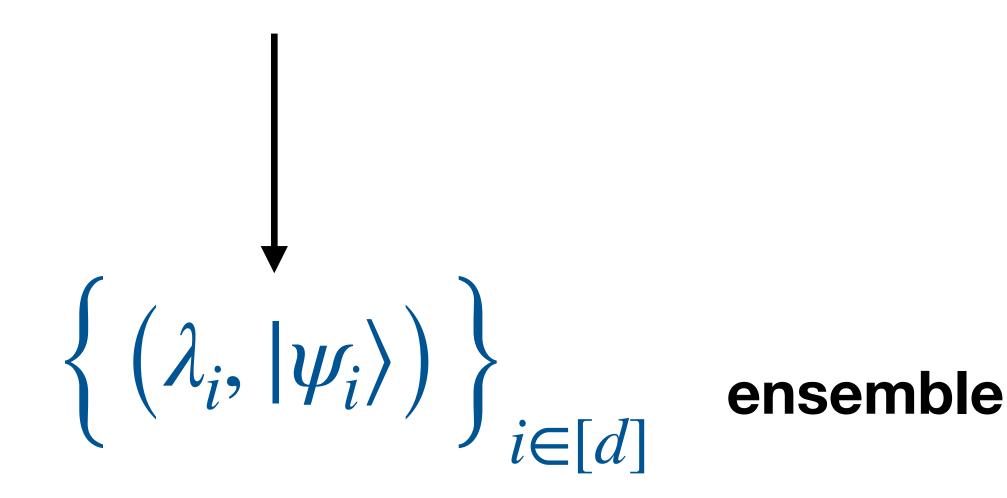
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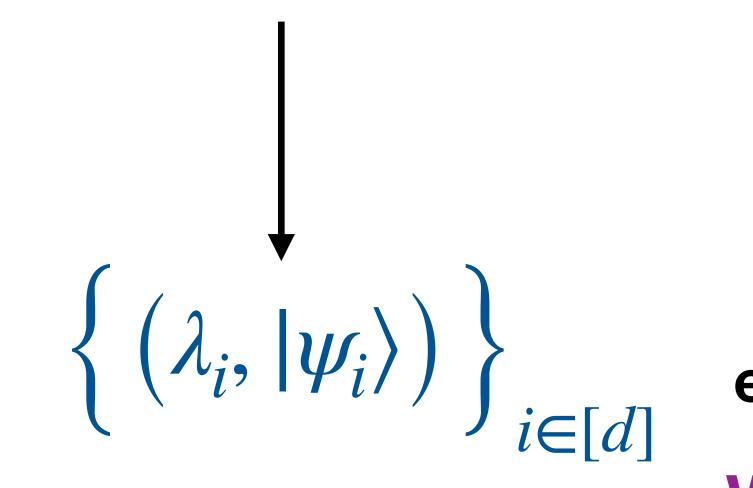
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ensemble

Why valid?

Given a density operator $\rho \in \mathbb{C}^{d \times d}$, can we find a corresponding ensemble?

Invoking the Spectral Theorem...

(1)
$$\operatorname{Tr}(\rho) = \sum_{i=1}^{d} \lambda_i = 1$$

$$\rho = \sum_{i=1}^d \lambda_i |\psi_i\rangle \langle \psi_i|$$

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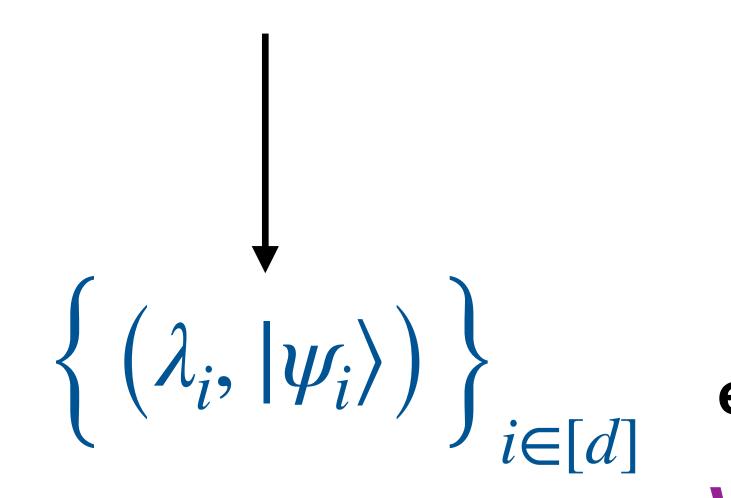
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(3)
$$\rho \ge 0 \implies \lambda_i \ge 0, \forall i \in [d]$$

$$\rho = \sum_{i=1}^{d} \lambda_i |\psi_i\rangle\langle\psi_i|$$



ensemble

Why valid?

Unitary Evolution

Given unitary U, evolution is given by

$$\left\{ \left(\lambda_i, |\psi_i \rangle \right) \right\}_{i \in [d]} \mapsto_U \left\{ \left(\lambda_i, U | \psi_i \rangle \right) \right\}_{i \in [d]} \tag{Ensemble}$$

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(Ensemble)

$$\rho \mapsto_U U \rho U^{\dagger}$$

(Density Operator)

A measurement is defined by a collection
$$\{M_i=E_i^\dagger E_i\in\mathbb{C}^{d imes d}\}_{i\in[m]}$$
 of positive semi-definite (PSD) matrices sastisfying $\sum_{i=1}^m M_i=I$

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(2)
$$\sum_{i=1}^{m} M_i = I, \operatorname{Tr}(\rho) = 1 \implies \sum_{i=1}^{m} p_i = \operatorname{Tr}\left(\sum_{i=1}^{m} M_i \rho\right) = 1 \checkmark$$

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(we require an explicit factorization $M_i=E_i^\dagger E_i$ since $M_i=E_i^\dagger U^\dagger U E_i$ for any unitary U)

POVM Measurement

The collection $\{M_i\in\mathbb{C}^{d imes d}\}_{i\in[m]}$ of positive semi-definite (PSD) matrices sastisfying $\sum M_i=I$

$$\sum_{i=1}^{m} M_i = I$$

is called Positive Operator-Valued Measure (POVM)

(In this case we do not require an explicit factorization $M_i=E_i^\dagger E_i$)

Example of Measurement

Measuring in the computational basis $\{M_x=|x\rangle\langle x|\in\mathbb{C}^{2^n\times 2^n}\}_{x\in\{0,1\}^n}$

Suppose
$$\rho = |\psi\rangle\langle\psi|$$
, where $|\psi\rangle = \sum_{x\in\{0,1\}^n} \alpha_x |x\rangle$

Then, $p_x={\rm Tr}(M_x\rho)={\rm Tr}(|x\rangle\langle x|\rho)=\langle x|\rho|x\rangle=\langle x|\psi\rangle\langle\psi|x\rangle=|\alpha_x|^2$

Example of Measurement

Measuring Hamming weight parity

$$\left\{ M_{\text{even}} = \sum_{x \in \{0,1\}^n: |x| \equiv 0 \pmod{2}} |x\rangle\langle x|, M_{\text{odd}} = I - M_{\text{even}} \right\}$$

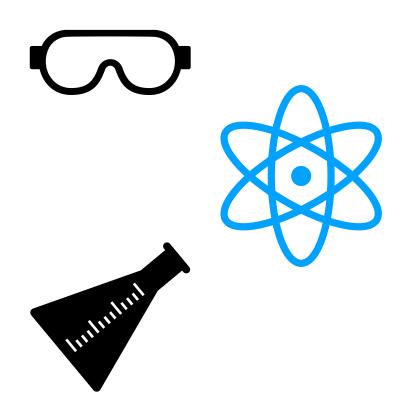
Suppose
$$\rho = |\psi\rangle\langle\psi|$$
, where $|\psi\rangle = \sum_{x\in\{0,1\}^n} \alpha_x |x\rangle$

Then,
$$p_{\text{even}} = \text{Tr}(M_{\text{even}}\rho) = \sum_{x \in \{0,1\}^n: |x| \equiv 0 \pmod 2} |\alpha_x|^2$$

How can we learn a quantum state?

Learning Scenario

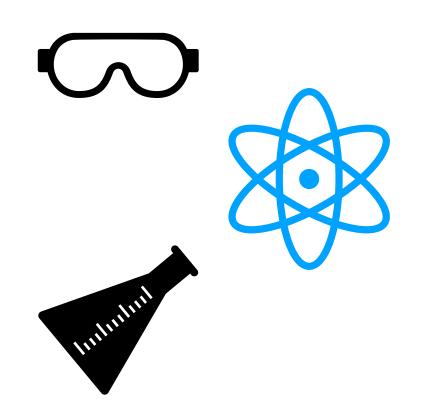
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What is the quantum state $\rho \in \mathbb{C}^{2\times 2}$?

Learning Scenario

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What is the quantum state $\rho \in \mathbb{C}^{2\times 2}$?

This task is called Quantum State Tomography

Hilbert-Schmidt Inner Product

Let $A, B \in \mathbb{C}^{d \times d}$. The Hibert-Schmidt inner product betwen A and B is defined as

$$\langle A, B \rangle = \operatorname{Tr}(A^{\dagger}B) = \sum_{i=1}^{d} \sum_{j=1}^{d} \overline{A_{i,j}} B_{i,j}$$

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(this is the entrywise inner product of the matrices)

Widely used matrices in Quantum Information Sciences in many contexts

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

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

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

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 phase flip error

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 bit and phase flip erros

Some Properties

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Given an arbitrary Hermitian matrix $H\in\mathbb{C}^{2\times 2}$, $H=\begin{pmatrix}a&b-ic\\b+ic&d\end{pmatrix}$, we have

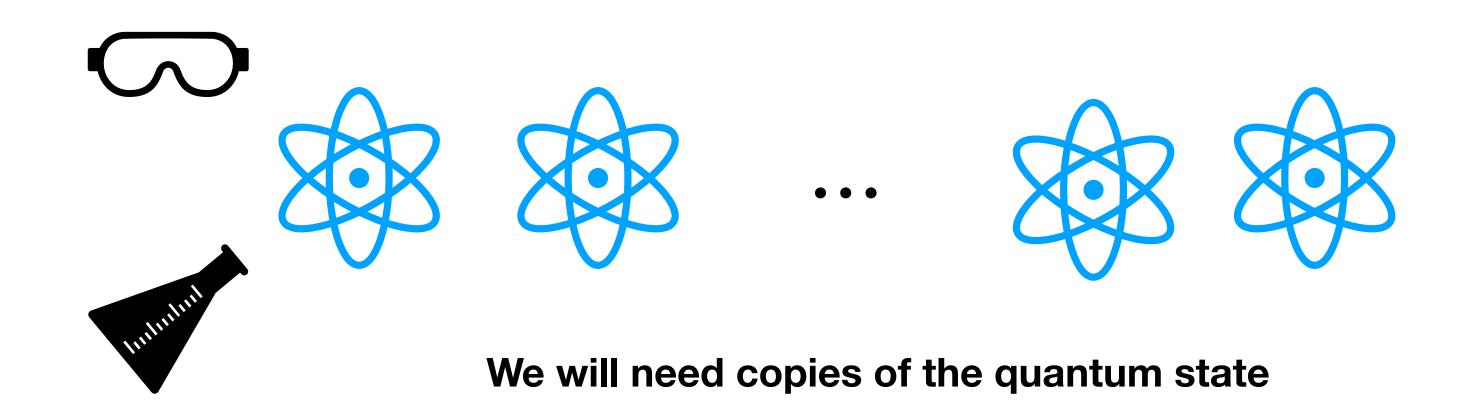
$$H = \frac{(a+d)}{2}I + bX + cY + \frac{(a-d)}{2}Z$$

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

The matrices $\{I,X,Y,Z\}$ form an orthogonal basis for the space of Hermitian matrices in $\mathbb{C}^{2 imes 2}$

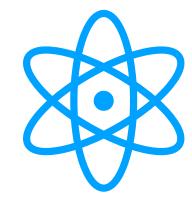
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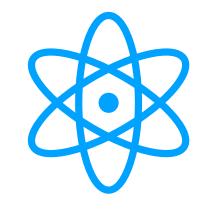
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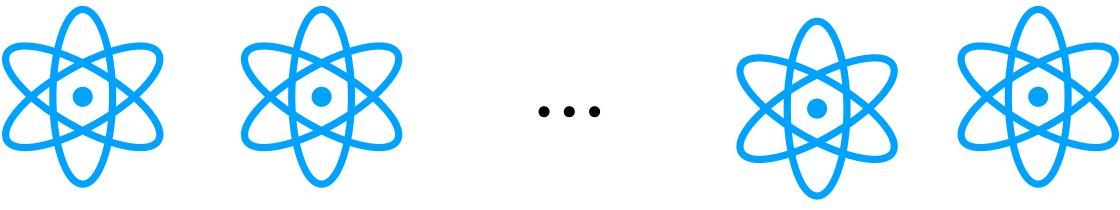


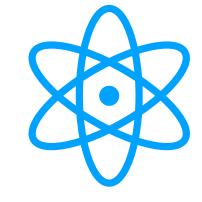
What is the quantum state $\rho \in \mathbb{C}^{2\times 2}$?

$$\rho = \begin{pmatrix} \rho_{1,1} & \rho_{1,2} \\ \rho_{2,1} & \rho_{2,2} \end{pmatrix}$$









We will need copies of the quantum state

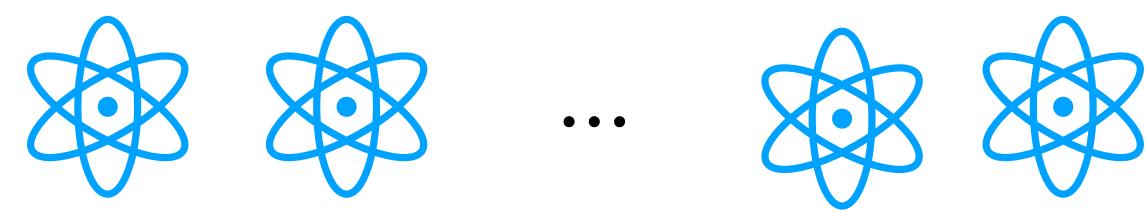
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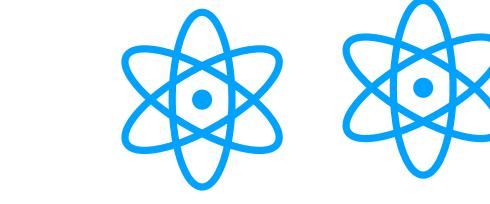
Using these copies, we estimate:

$$a_{x} = \langle X, \rho \rangle \approx \hat{a}_{x}$$

$$a_{y} = \langle Y, \rho \rangle \approx \hat{a}_{y}$$

$$a_z = \langle Z, \rho \rangle \approx \hat{a}_z$$



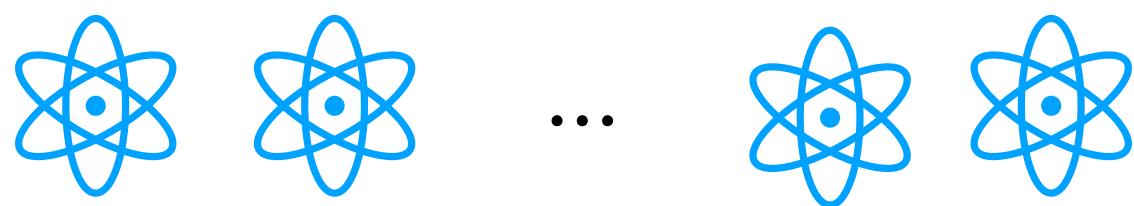


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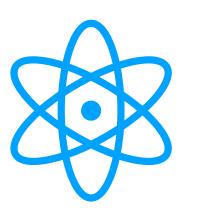
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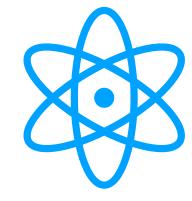
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 $\rho = \frac{I + a_{x}X + a_{y}Y + a_{z}Z}{2}$
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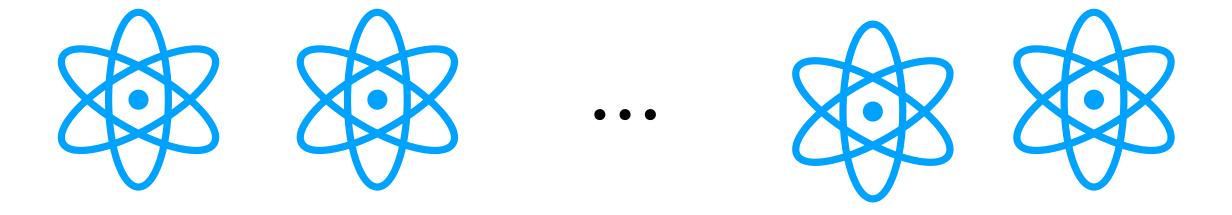
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Output the approximation

$$\rho = \frac{I + a_x X + a_y Y + a_z Z}{2} \approx \hat{\rho} = \frac{I + \hat{a}_x X + \hat{a}_y Y + \hat{a}_z Z}{2}$$

How can we learn an n-qubit state?

What is the quantum state $\rho \in \mathbb{C}^{2^n \times 2^n}$?



We will need maaaaa...any copies of the quantum state for n large!

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What is the quantum state $\rho \in \mathbb{C}^{2^n \times 2^n}$?

The matrices $\{I,X,Y,Z\}^{\otimes n}$ form an orthogonal basis for the space of Hermitian matrices in $\mathbb{C}^{2^n \times 2^n}$

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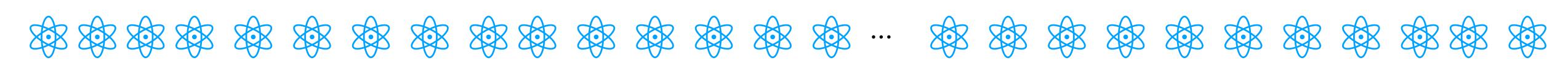
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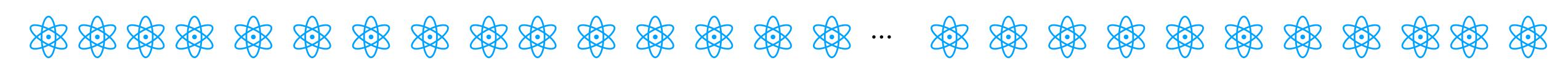
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Can we hope to learn a good approximation of a 300-qubit state in general?

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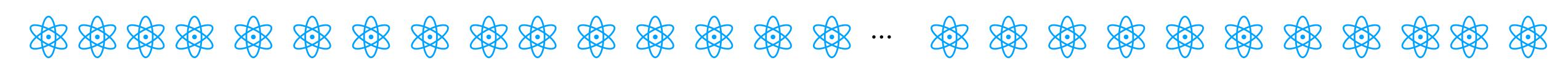


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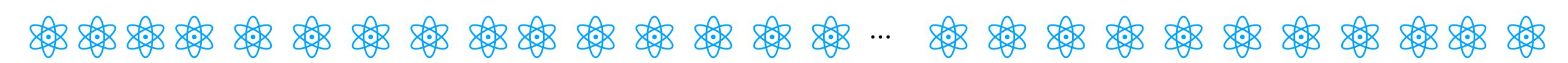
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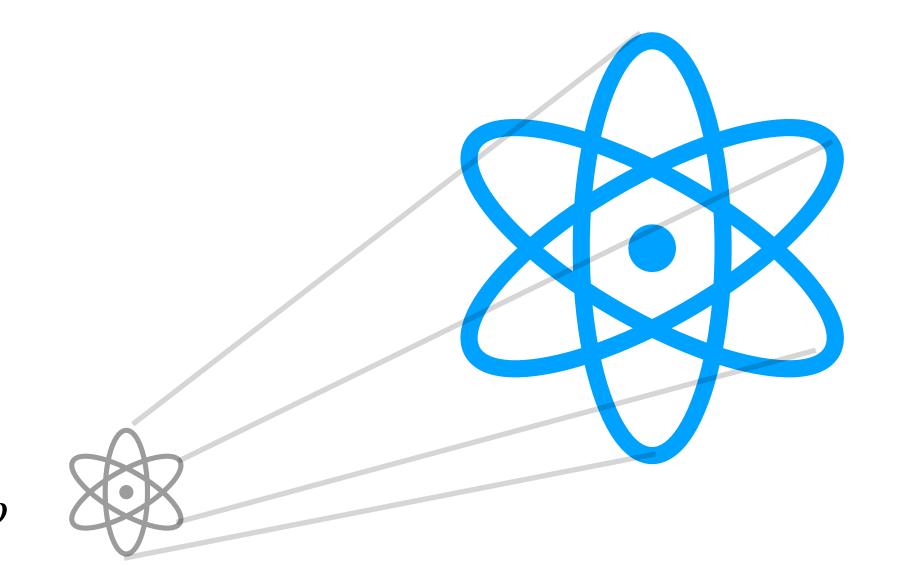
Should we simply give up?

No! Many notions of cheaper tomography known as Shadow Tomography!

A Glimplse of an Active Research Topic: The Shadow Tomography Case

What if instead of learning an entire n-qubit state we learn just enough to determine many properties of the quantum state?

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Quantum state $\rho \in \mathbb{C}^{2^n \times 2^n}$

Shadow of ρ

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Say that we have a large collection of binary (two-outcome) POVM $\{M_i\}_{i\in[m]}$ (representing our properties of interest)

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Goal: Given copies of $\rho \in \mathbb{C}^{d \times d}$ and precision parameter $\epsilon > 0$, estimate $\langle M_i, \rho \rangle \pm \epsilon, \forall i \in [m]$

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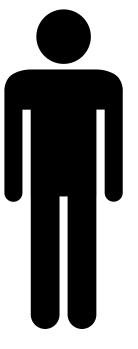
Amazing: In particular, we can learn $4^{\Theta(n)}$ properties (as above) of n-qubit states with only $n^{O(1)}$ copies!

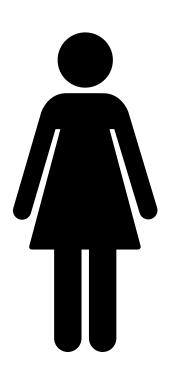
There are many variants of Shadow tomography extending the seminal work of Aaronson with various guarantees

(this is an active research area)

Back to Alice in Scenario 1







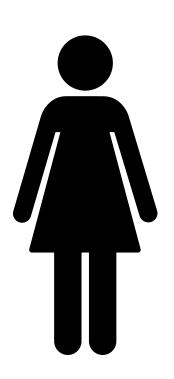


$$|\mathbf{EPR}\rangle = \frac{1}{\sqrt{2}}|0\rangle^A|0\rangle^B + \frac{1}{\sqrt{2}}|1\rangle^A|1\rangle^B$$





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What is the state of Alice's quantum system?

$$|\mathbf{EPR}\rangle = \frac{1}{\sqrt{2}}|0\rangle^A|0\rangle^B + \frac{1}{\sqrt{2}}|1\rangle^A|1\rangle^B \neq |\psi_A\rangle \otimes |\psi_B\rangle$$

(no matter the choice of $|\psi_A\rangle$, $|\psi_B\rangle$)



What is the state of Alice's quantum system?

It is not a pure state!

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What is the state of Alice's quantum system?

It is not a pure state!

It is a mixed state given by a density operator!

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How can we compute the density operator on Alice's quantum sub-system?

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We will need the partial trace operation!

Sub-system State via Partial Trace

Let $\rho_{AB} \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$ be a density operator on a bipartite tensor space

 $\mathcal{H}_A \otimes \mathcal{H}_B$ with orthornomal basis $\{|i\rangle_A\}_{i\in[d_A]}$ and $\{|i\rangle_B\}_{i\in[d_B]}$

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The reduced density operator ho_A on subsystem A is given by the partial trace ${
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where the partial trace ${\sf Tr}_B(\ \cdot\)$ is the linear operator acting on basis elements as

$$\mathbf{Tr}_{B}(|i_{A}\rangle\langle j_{A}|\otimes|i_{B}\rangle\langle j_{B}|) = |i_{A}\rangle\langle j_{A}|\mathbf{Tr}(|i_{B}\rangle\langle j_{B}|) = |i_{A}\rangle\langle j_{A}|\langle j_{B}|i_{B}\rangle\langle j_{B}|)$$

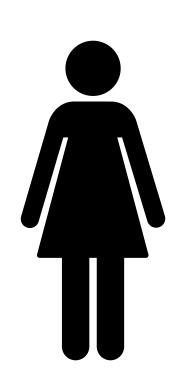
Alice's State via Partial Trace



$$|\mathbf{EPR}\rangle = \frac{1}{\sqrt{2}}|0\rangle^A|0\rangle^B + \frac{1}{\sqrt{2}}|1\rangle^A|1\rangle^B$$

$$\rho_{AB} = |\mathbf{EPR}\rangle\langle\mathbf{EPR}| = \frac{1}{2}|0\rangle^{A}|0\rangle^{B}\langle0|^{A}\langle0|^{B} + \frac{1}{2}|1\rangle^{A}|1\rangle^{B}\langle0|^{A}\langle0|^{B} + \frac{1}{2}|0\rangle^{A}|0\rangle^{B}\langle1|^{A}\langle1|^{B} + \frac{1}{2}|1\rangle^{A}|1\rangle^{B}\langle1|^{A}\langle1|^{B}$$

Alice's State via Partial Trace



$$|\mathbf{EPR}\rangle = \frac{1}{\sqrt{2}}|0\rangle^A|0\rangle^B + \frac{1}{\sqrt{2}}|1\rangle^A|1\rangle^B$$

$$\begin{split} \rho_A &= \operatorname{Tr}_B(\rho_{AB}) \\ &= \frac{1}{2} \operatorname{Tr}_B(|0\rangle^A |0\rangle^B \langle 0|^A \langle 0|^B) + \frac{1}{2} \operatorname{Tr}_B(|1\rangle^A |1\rangle^B \langle 0|^A \langle 0|^B) \\ &+ \frac{1}{2} \operatorname{Tr}_B(|0\rangle^A |0\rangle^B \langle 1|^A \langle 1|^B) + \frac{1}{2} \operatorname{Tr}_B(|1\rangle^A |1\rangle^B \langle 1|^A \langle 1|^B) \\ &= \frac{1}{2} |0\rangle^A \langle 0|^A + \frac{1}{2} |1\rangle^A \langle 1|^A \end{split}$$

Alice's State via Partial Trace



$$|\mathbf{EPR}\rangle = \frac{1}{\sqrt{2}}|0\rangle^A|0\rangle^B + \frac{1}{\sqrt{2}}|1\rangle^A|1\rangle^B$$

$$= \frac{1}{2} \operatorname{Tr}_{B}(|0\rangle^{A}|0\rangle^{B}\langle 0|^{A}\langle 0|^{B}) + \frac{1}{2} \operatorname{Tr}_{B}(|1\rangle^{A}|1\rangle^{B}\langle 0|^{A}\langle 0|^{B}) + \frac{1}{2} \operatorname{Tr}_{B}(|0\rangle^{A}|0\rangle^{B}\langle 1|^{A}\langle 1|^{B}) + \frac{1}{2} \operatorname{Tr}_{B}(|1\rangle^{A}|1\rangle^{B}\langle 1|^{A}\langle 1|^{B}) + \frac{1}{2} \operatorname{Tr}_{B}(|1\rangle^{A}|1\rangle^{B}\langle 1|^{A}\langle 1|^{B})$$

 $= \frac{1}{2}|0\rangle^A\langle 0|^A + \frac{1}{2}|1\rangle^A\langle 1|^A$

Maximally mixed state!

Due to entanglement between Alice and Bob, Alice reduced state is mixed!

What is quantum entanglement?

What is quantum entanglement?

(We will focus on bipartite entanglement of pure quantum states)

Thank you!

Thank you!

More Questions?