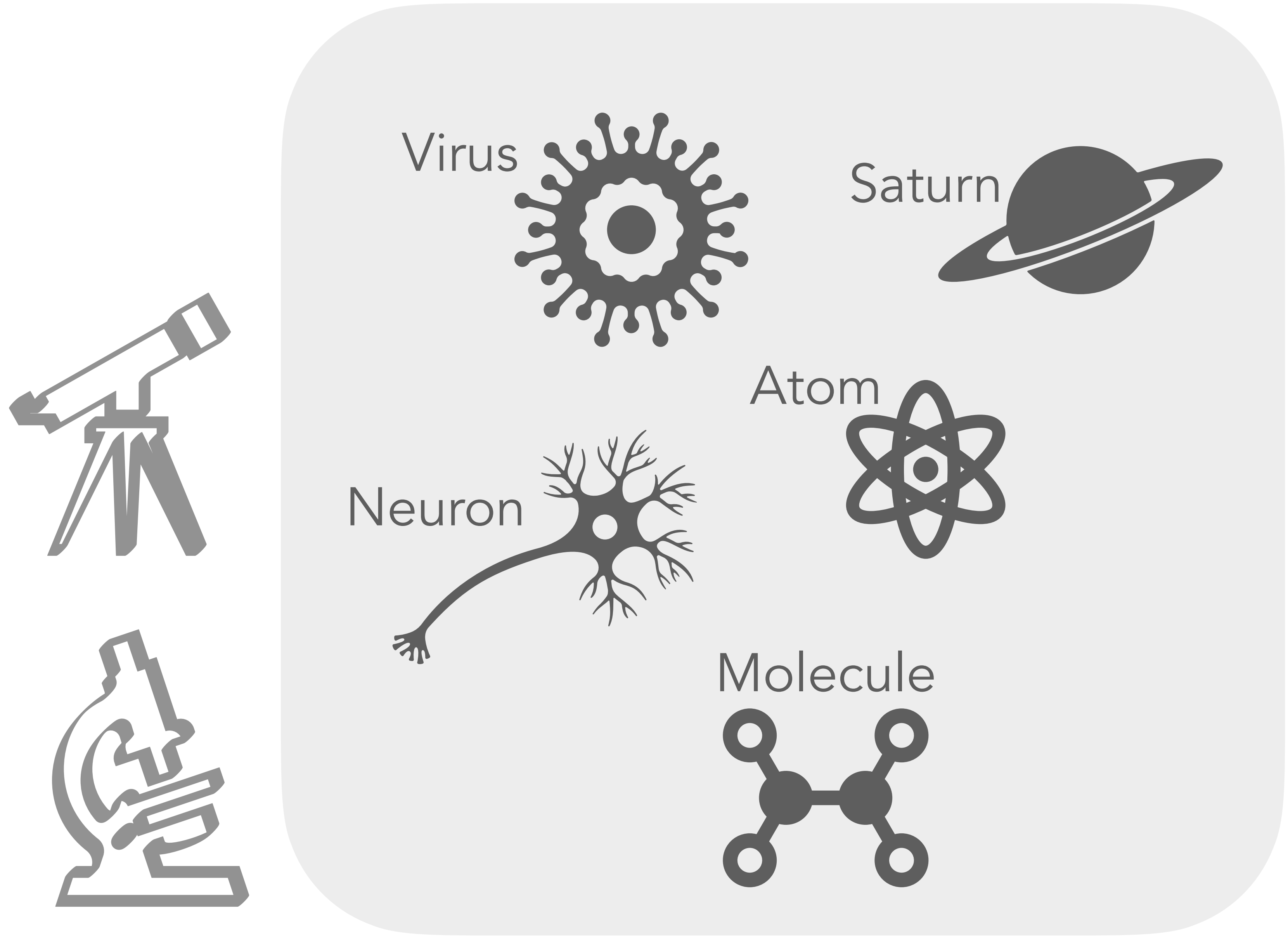
Tutorial: Quantum Learning & Certification

Hsin-Yuan Huang (Robert)

Assistant Professor of Theoretical Physics, Caltech (Starting March 2025)
Senior Research Scientist, Google Quantum AI

Motivation

- A central goal of science is to learn how our universe operates.



Examples of scientific disciplines

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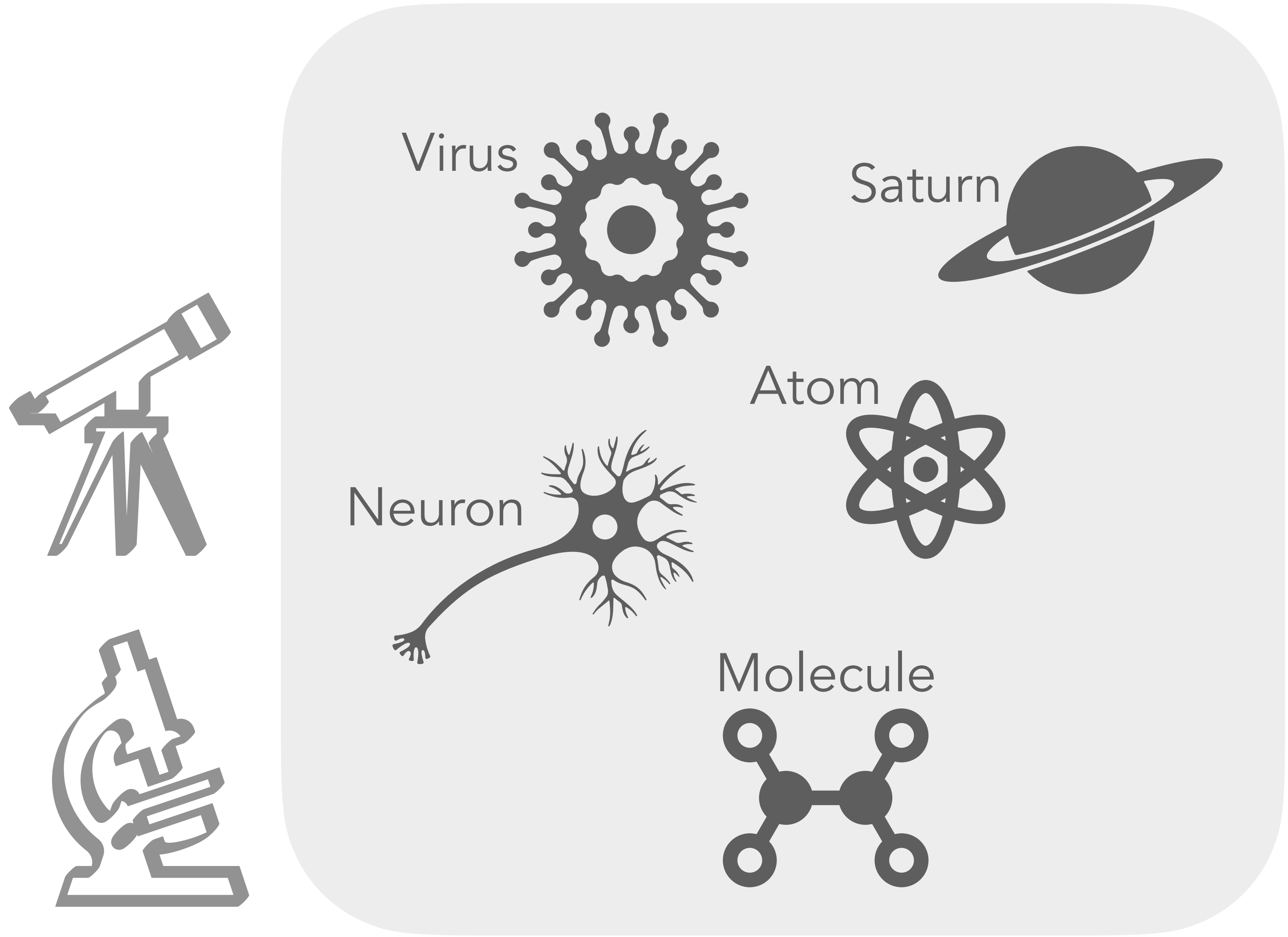

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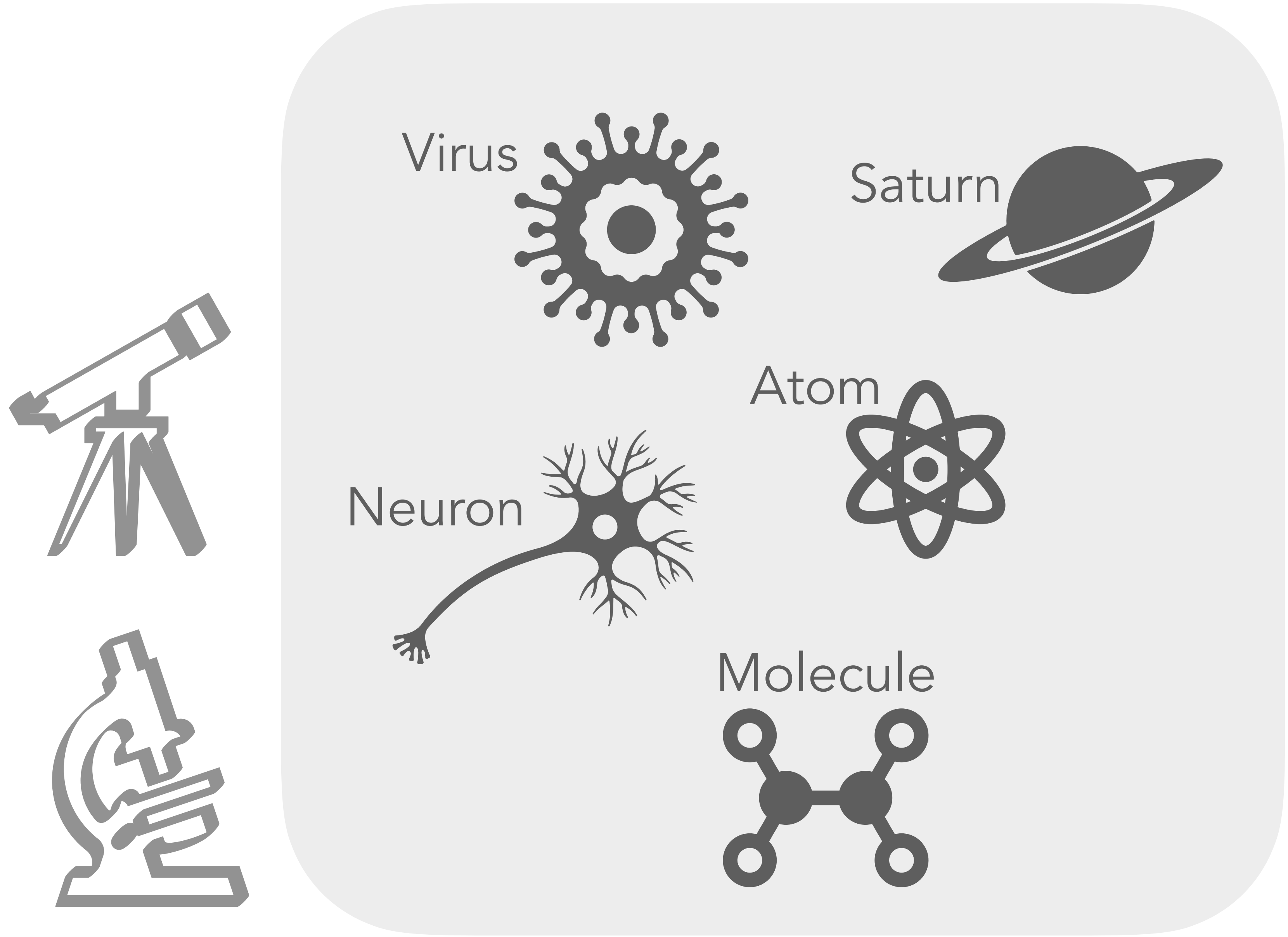

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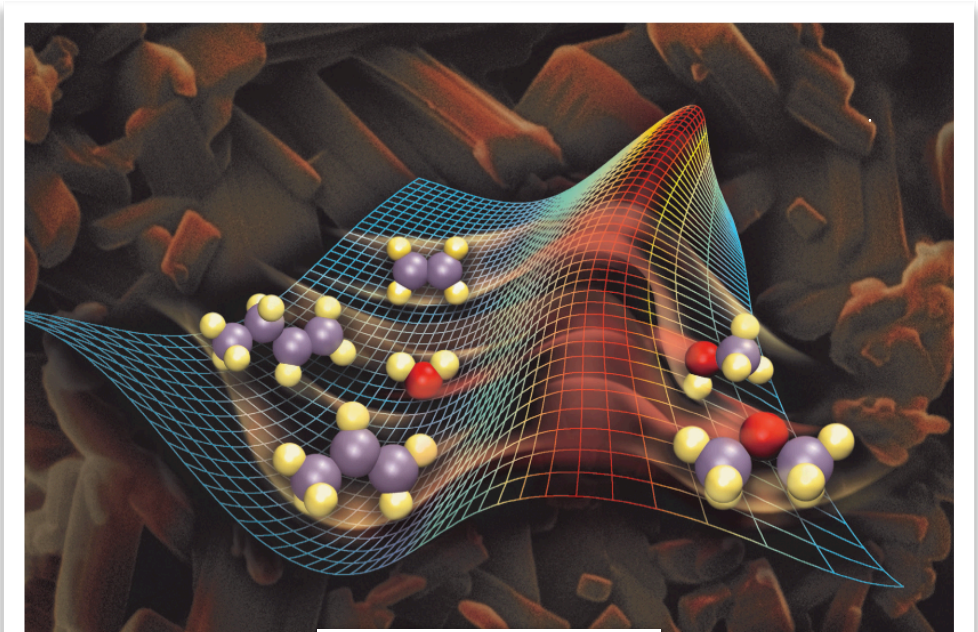

Catalysts

Pharmaceutics

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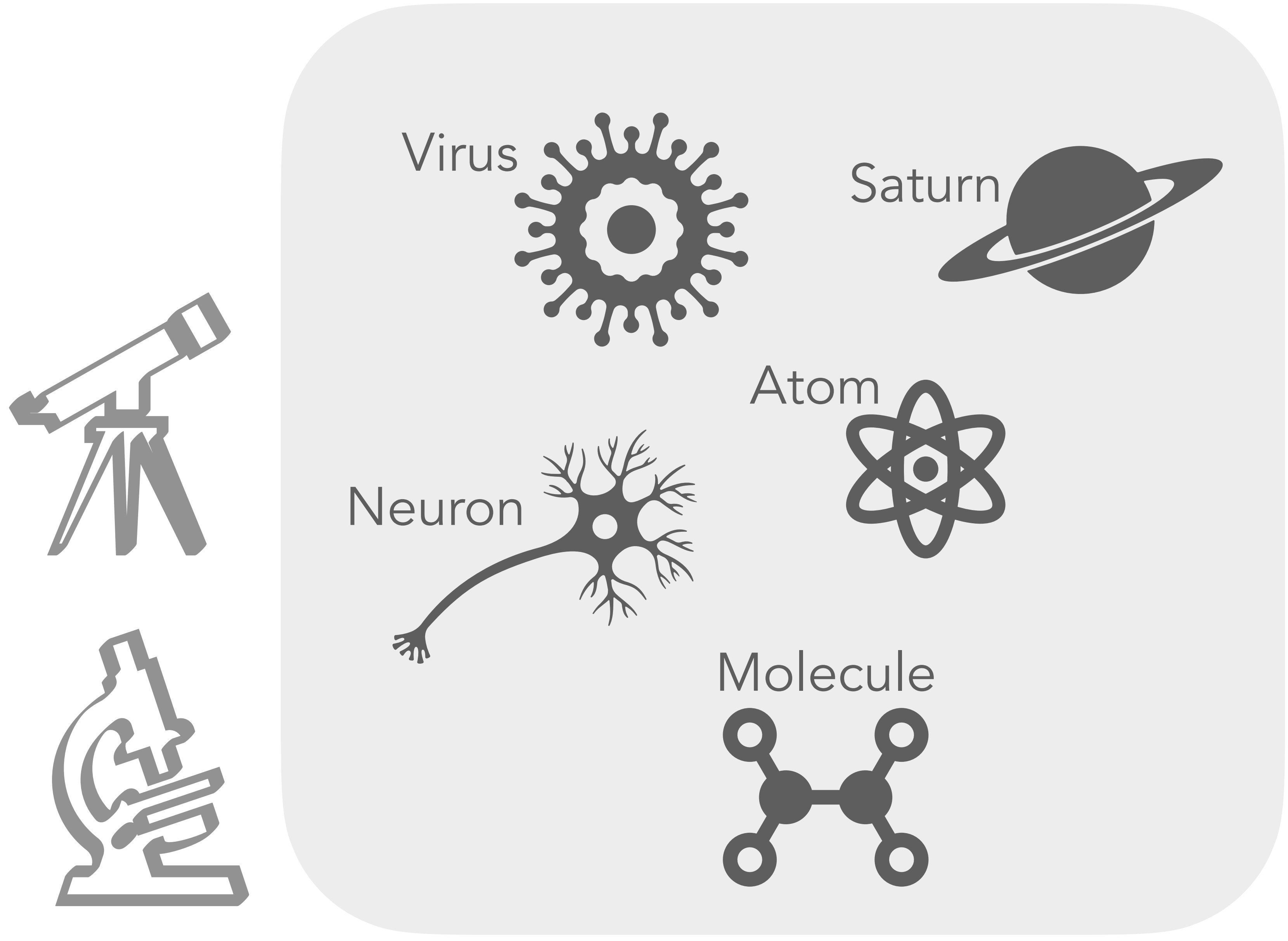

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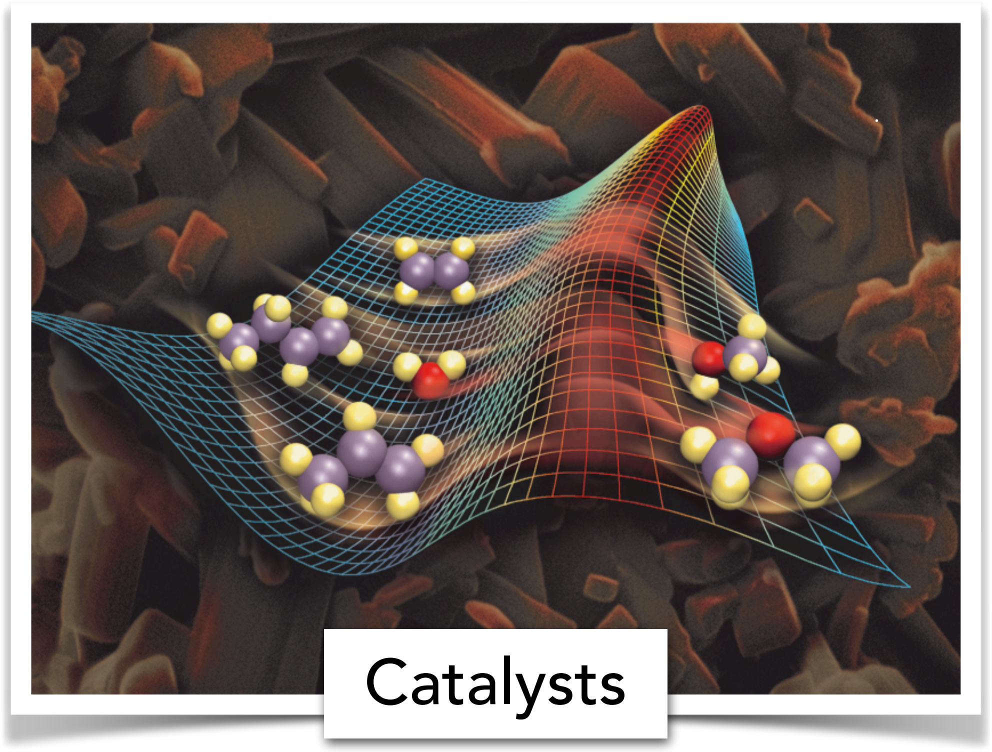

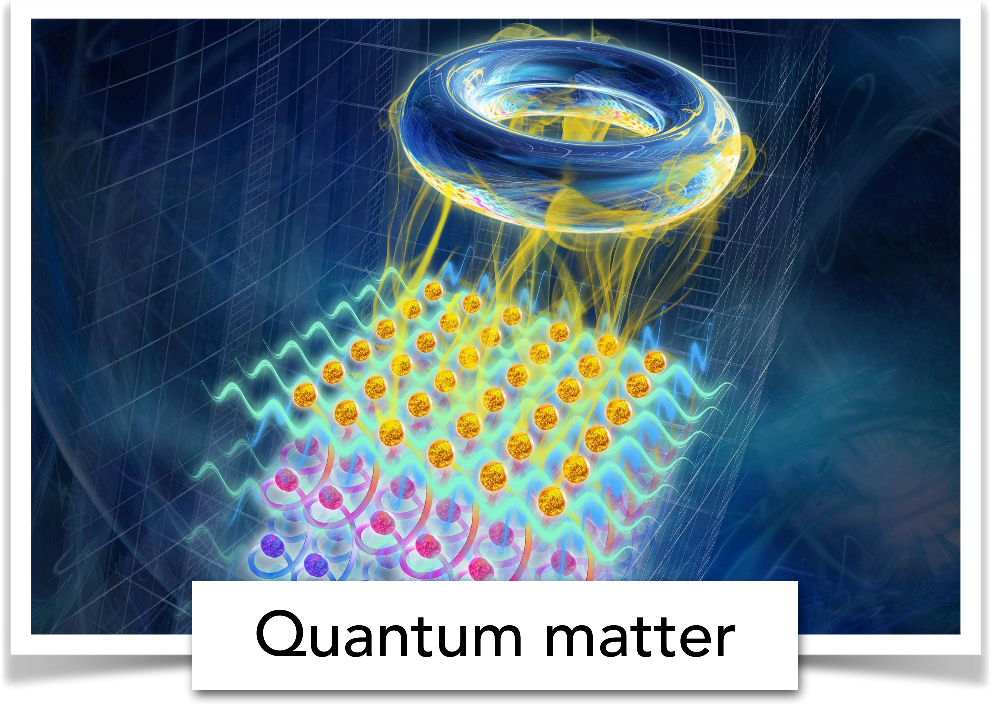

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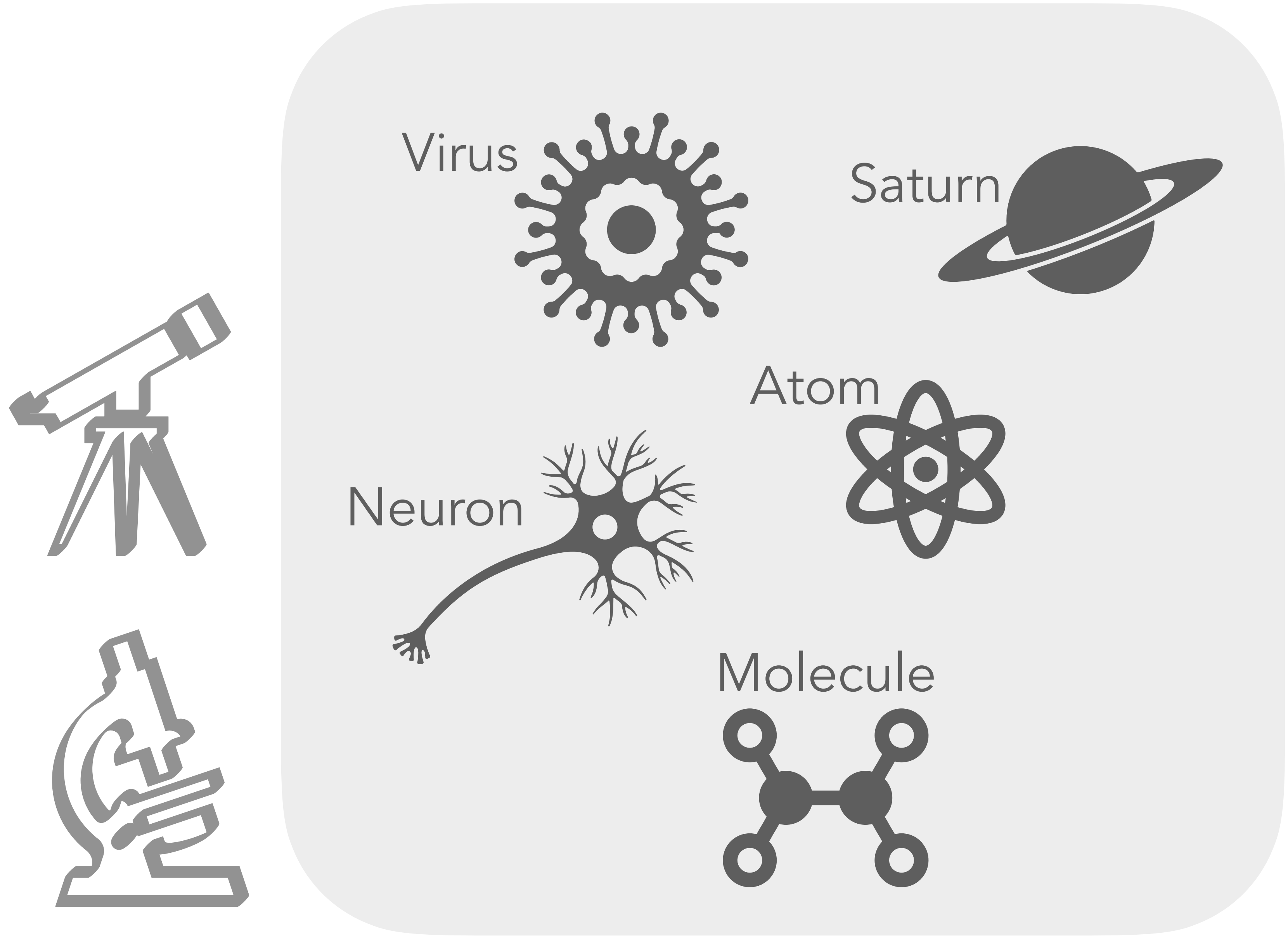

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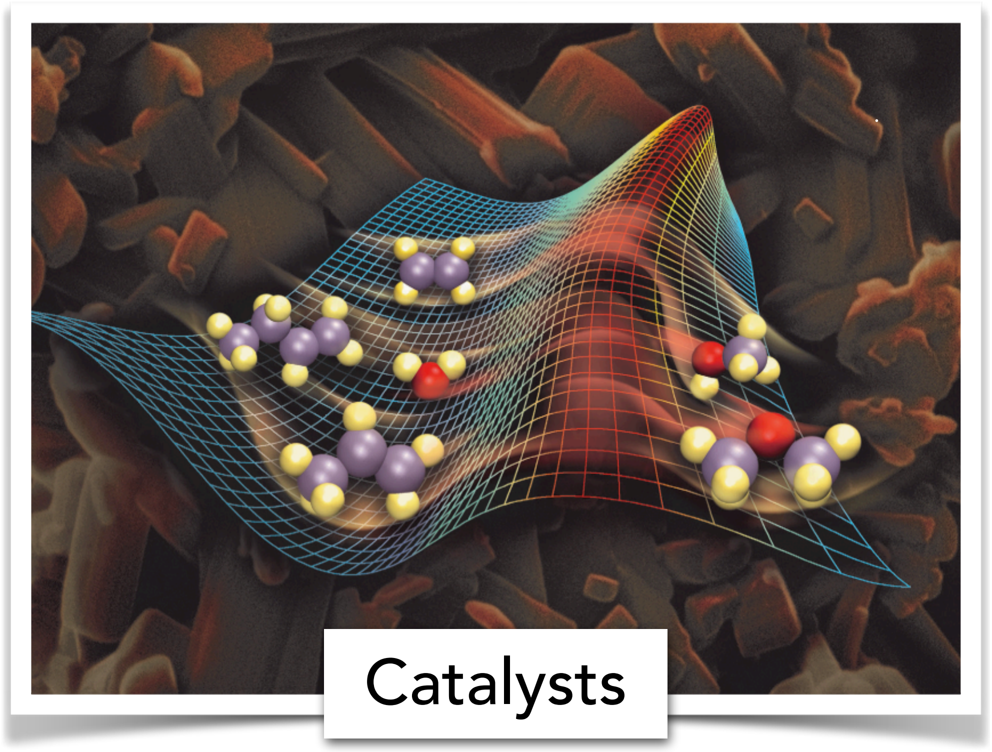

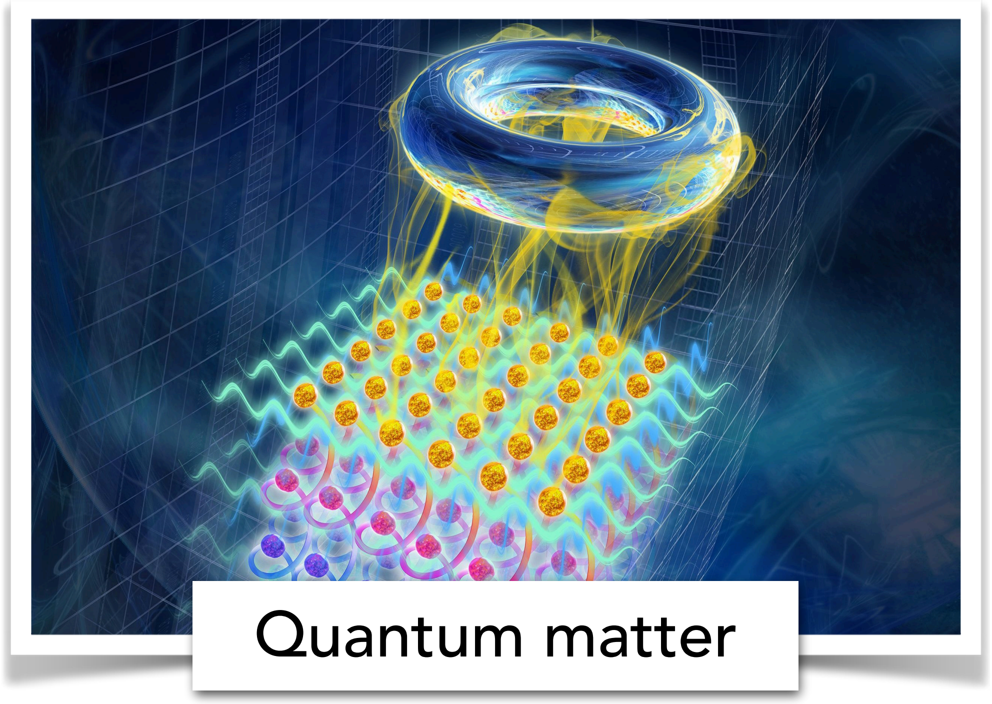

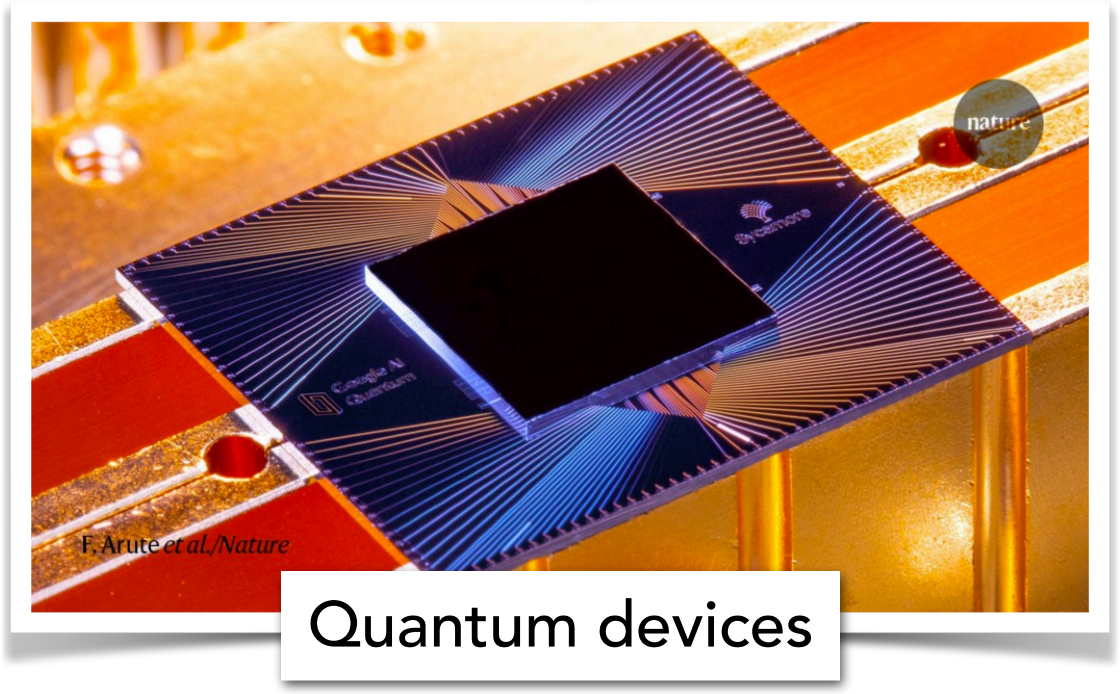

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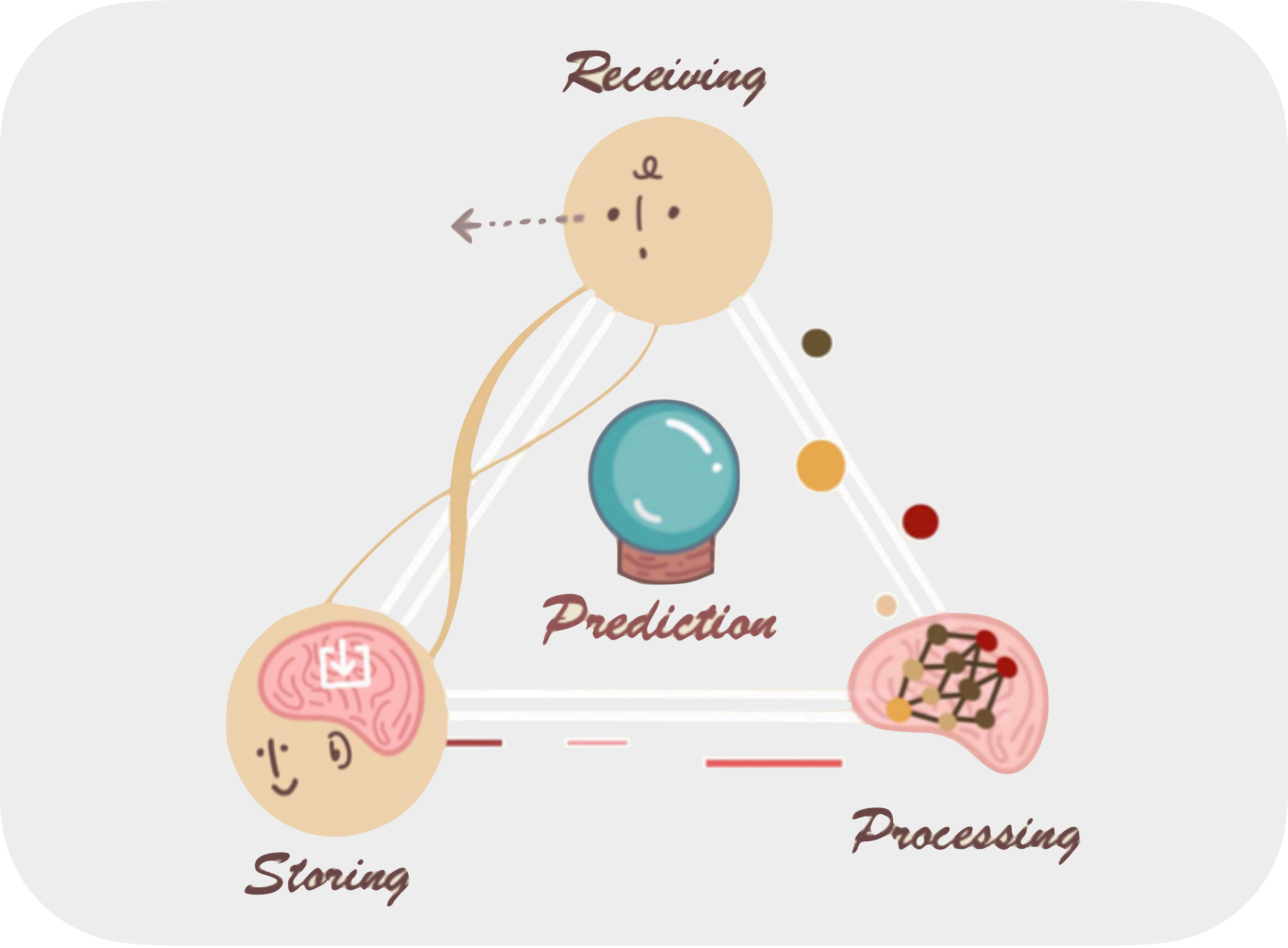

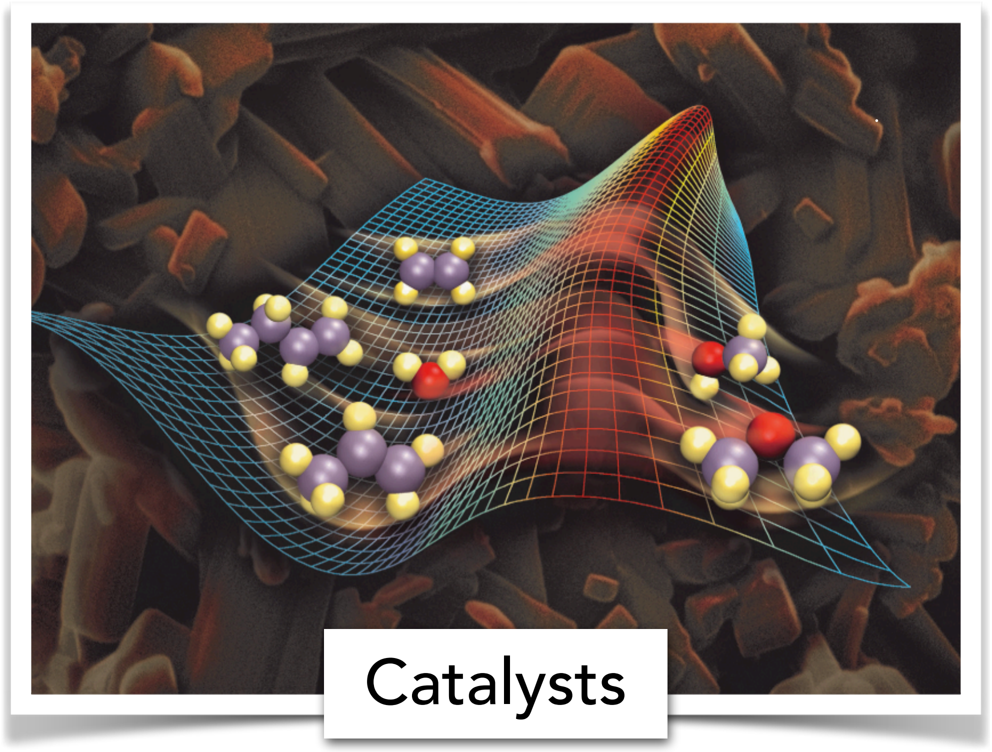
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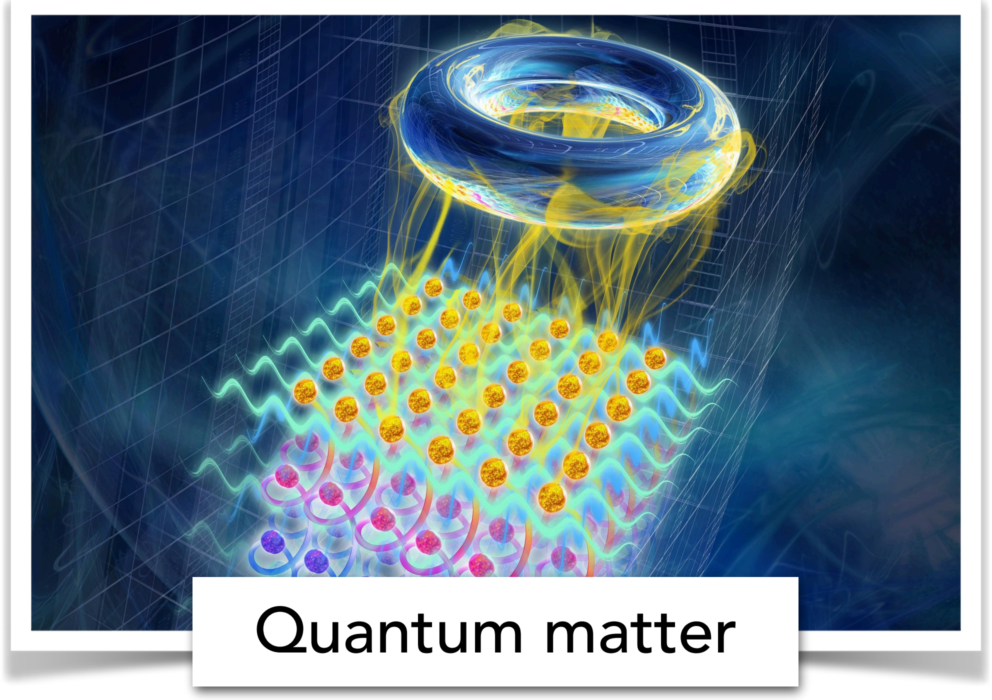
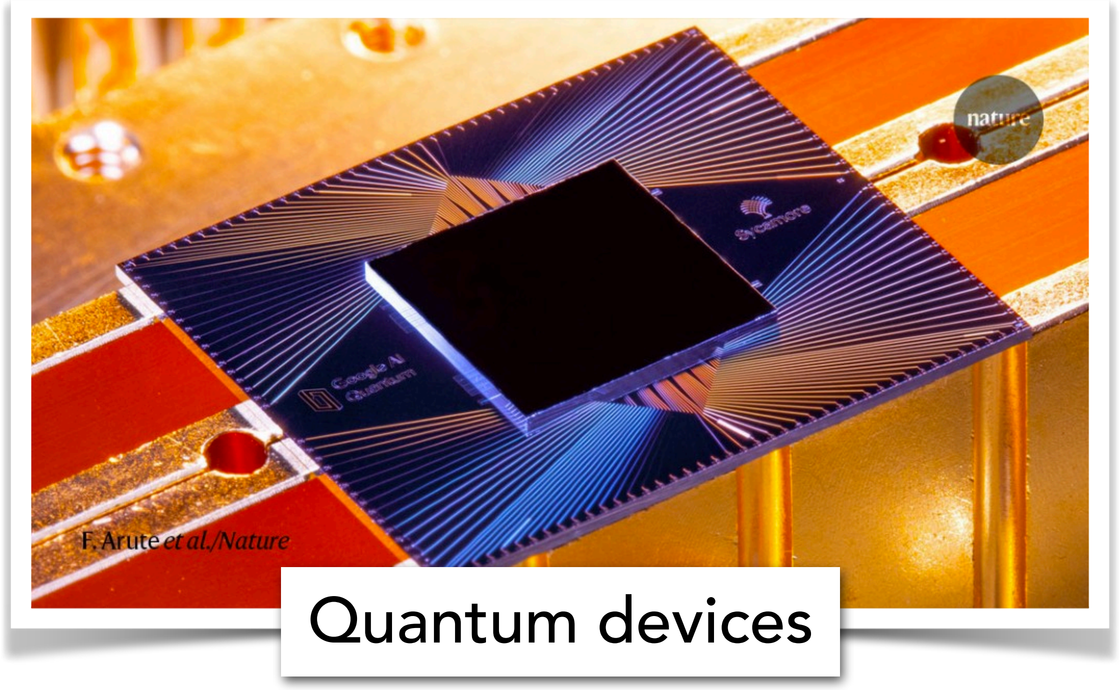

Quantum matter



Quantum devices

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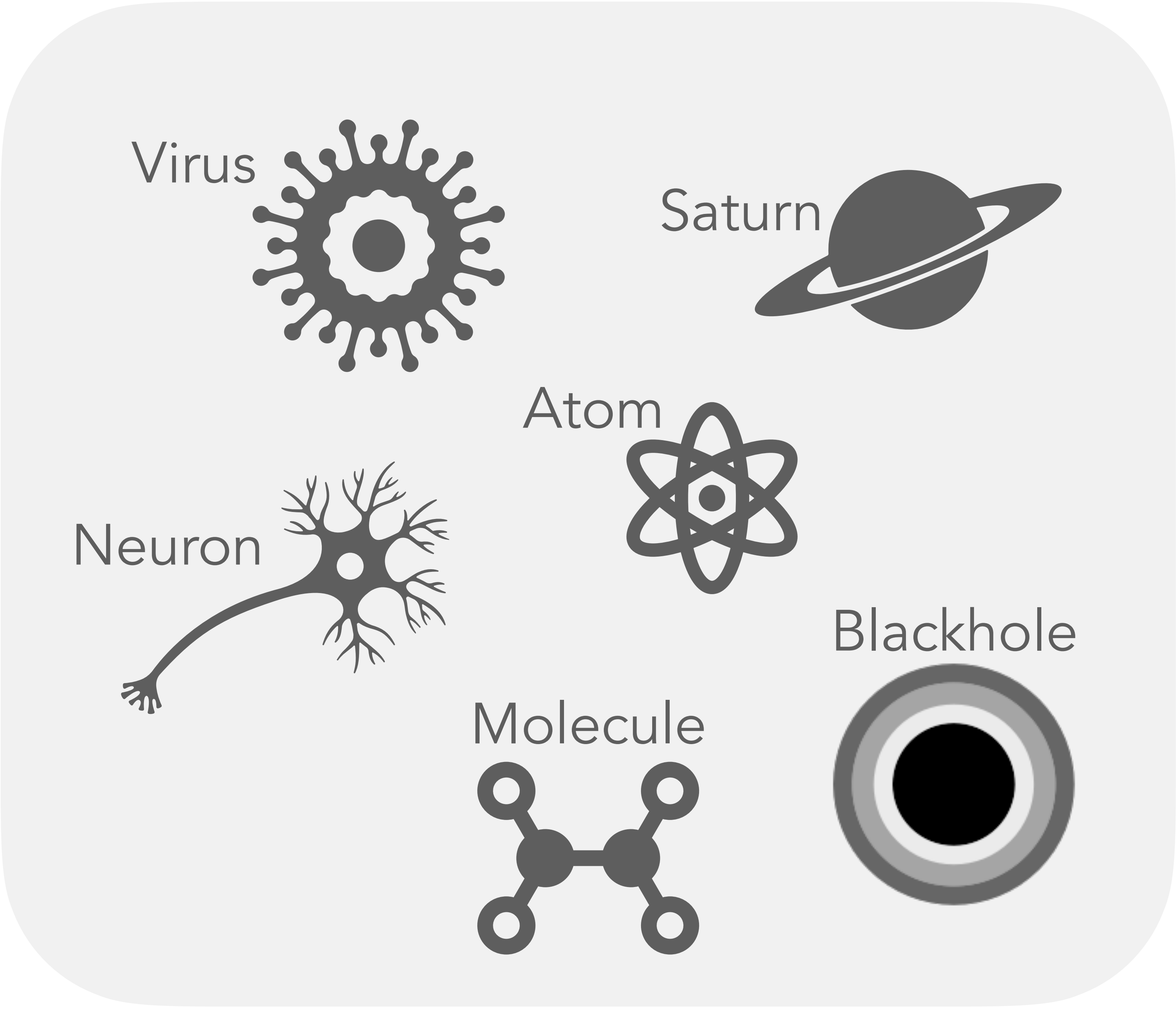
Definition: Learning



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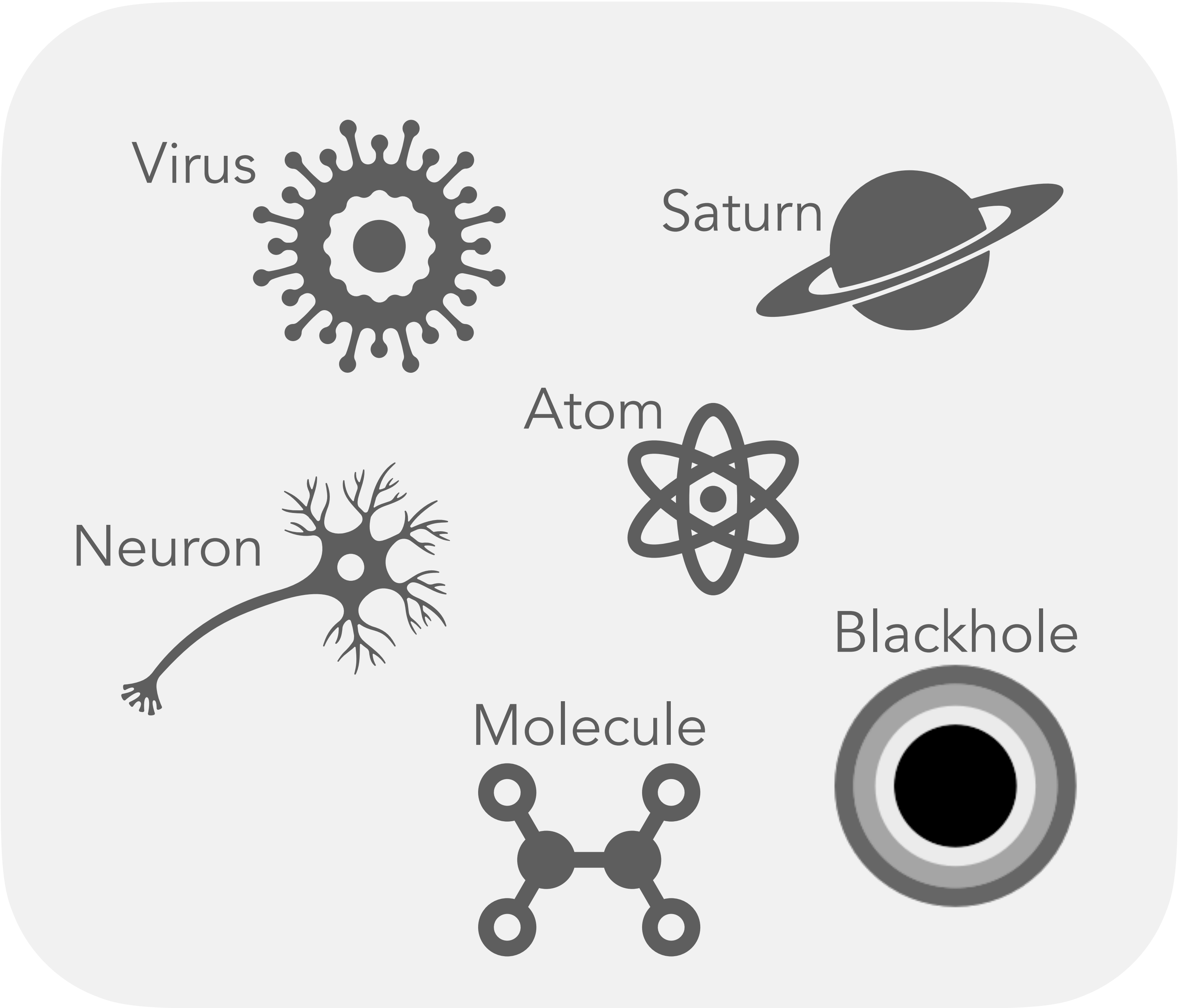

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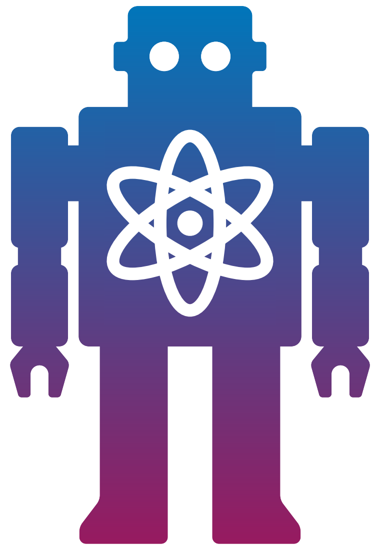
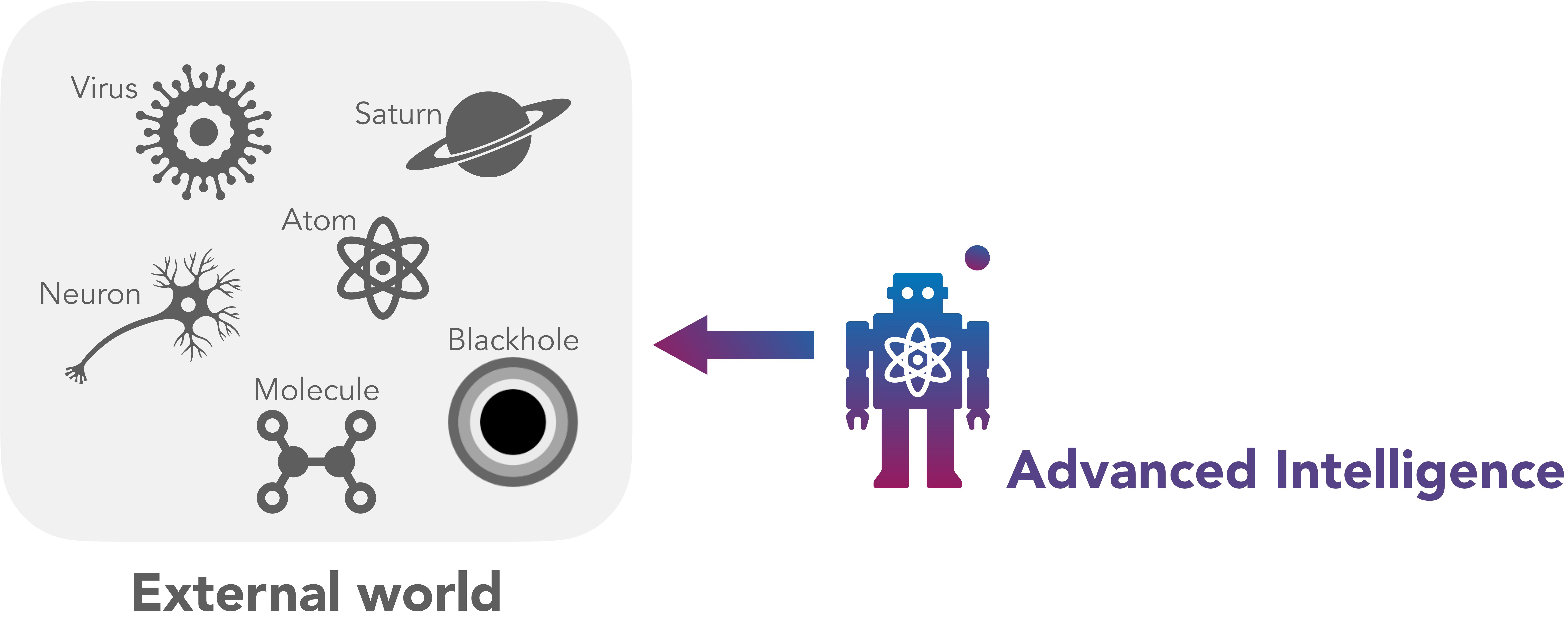


Advanced Intelligence

Definition: Learning



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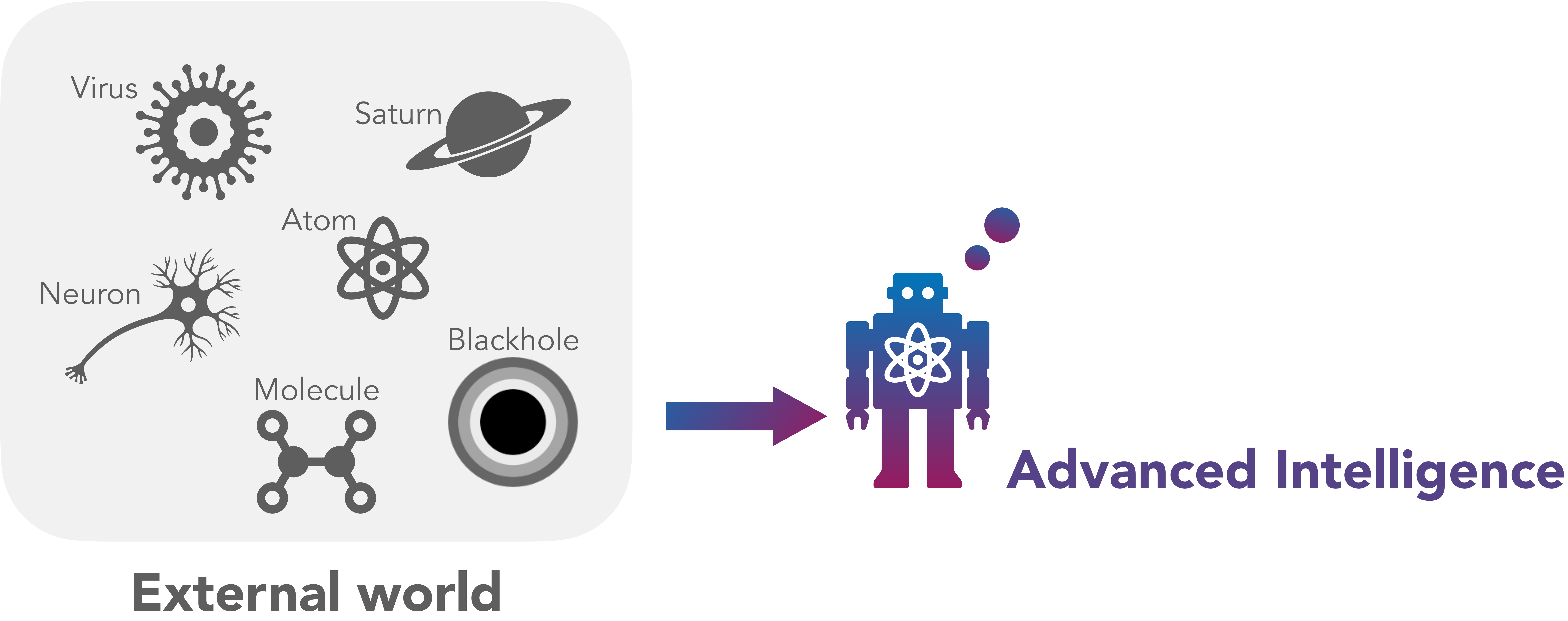

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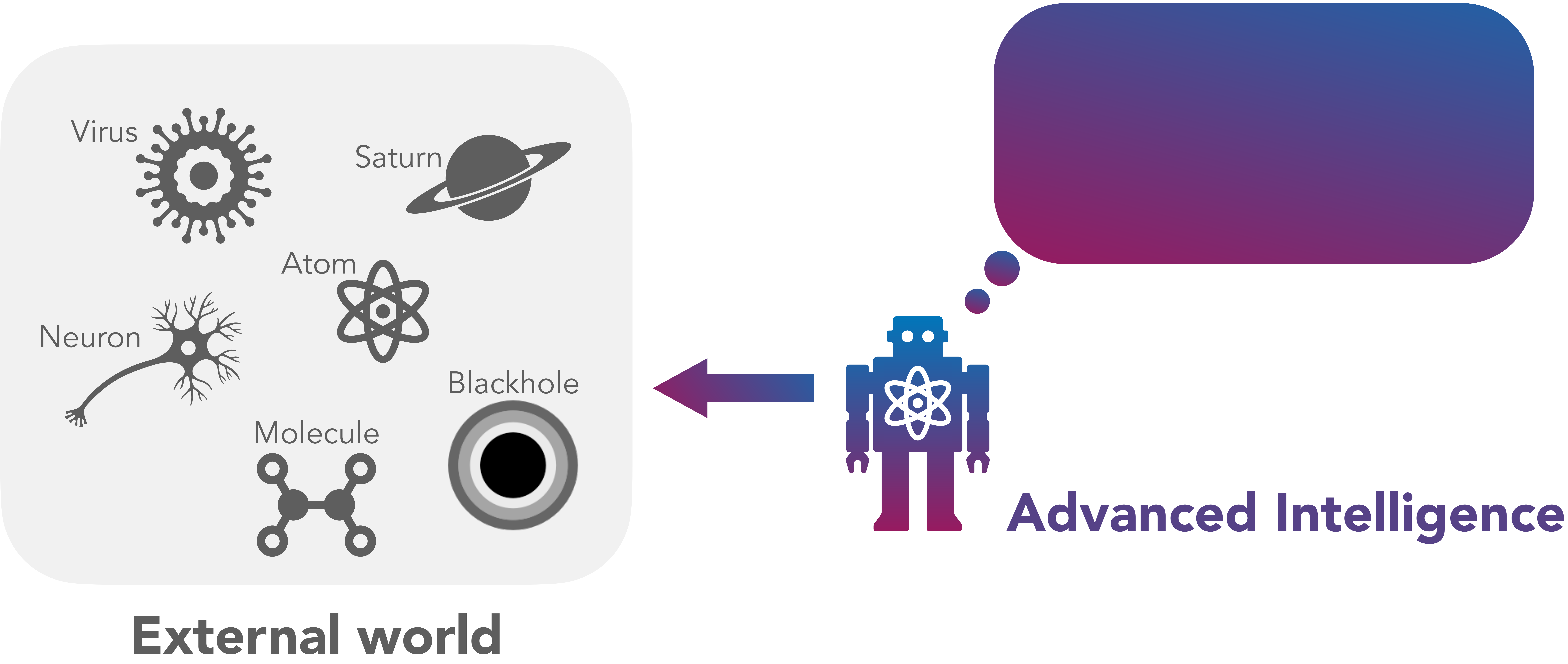

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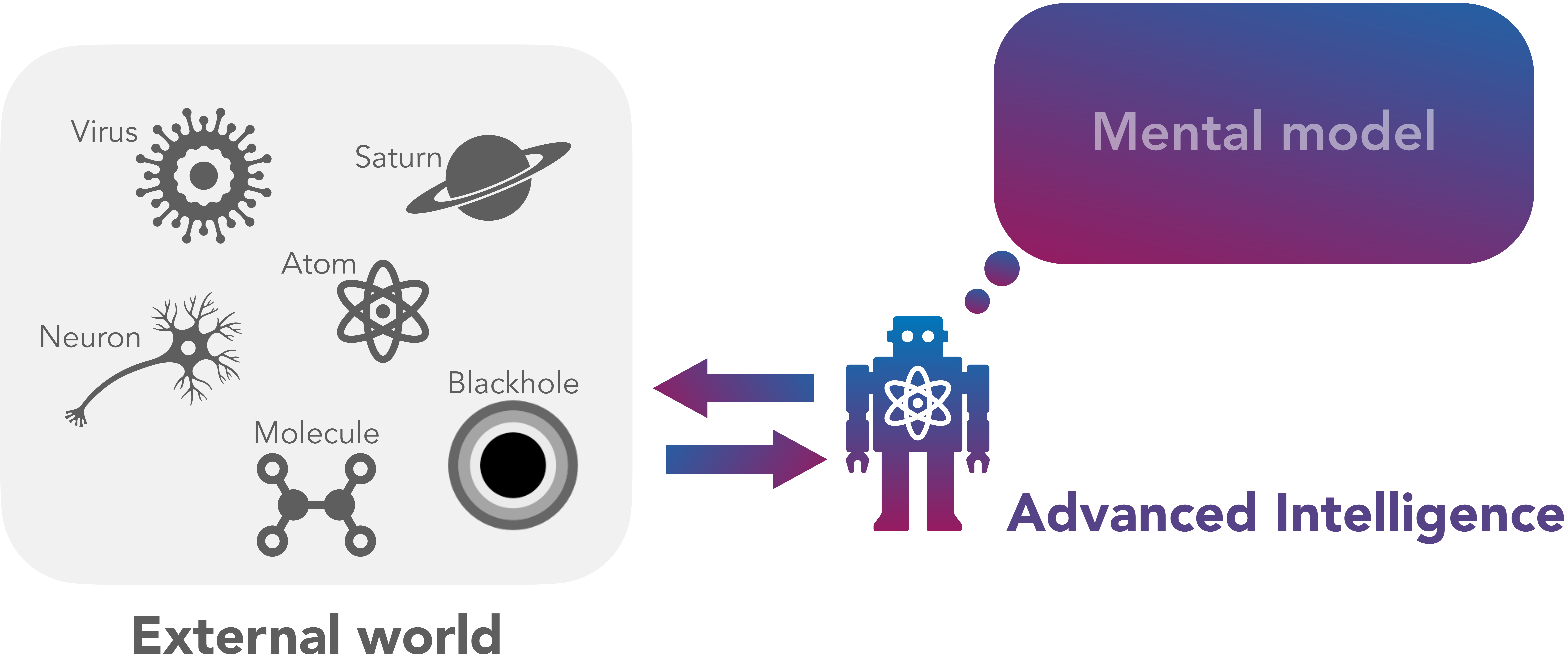

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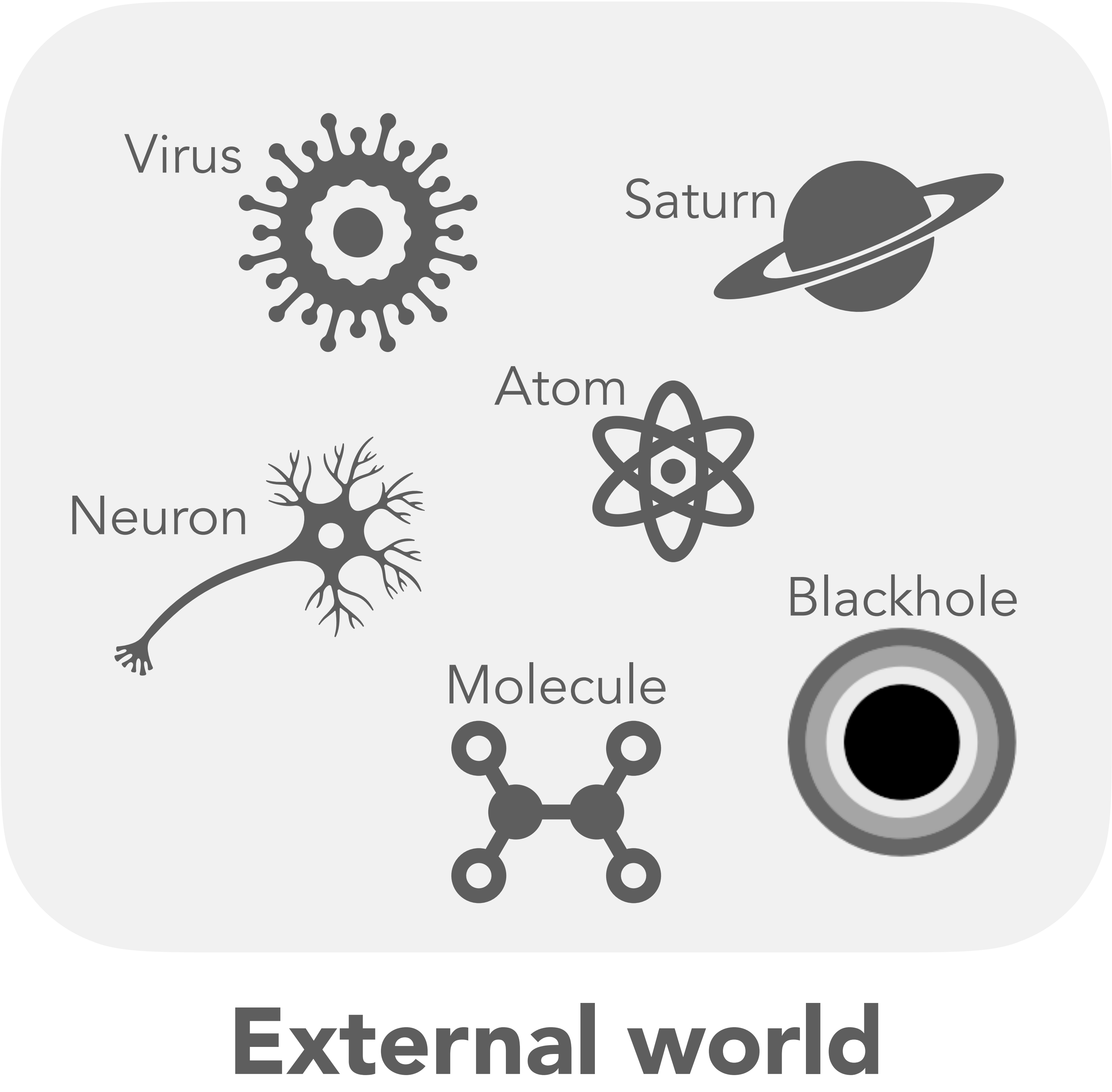

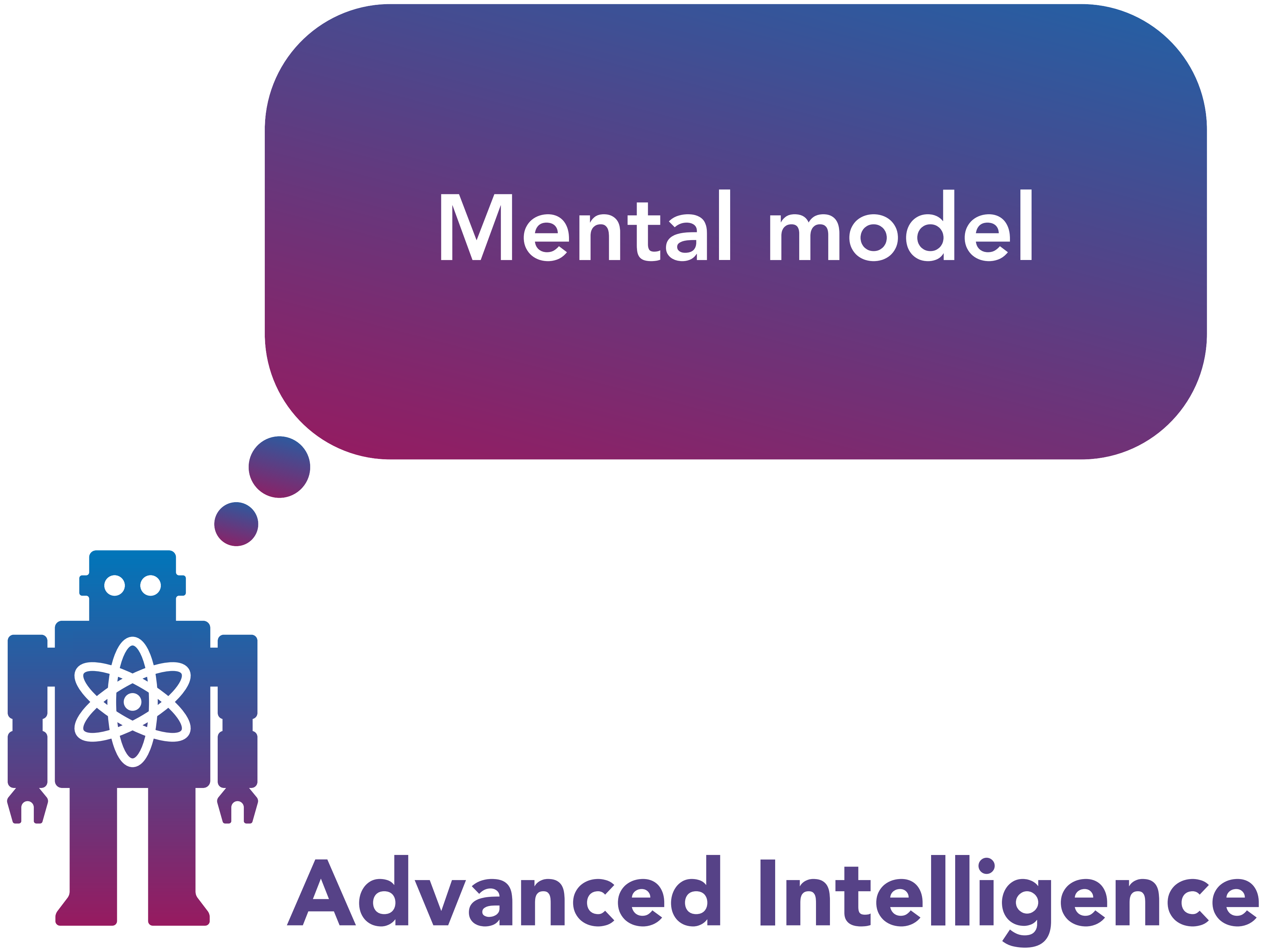

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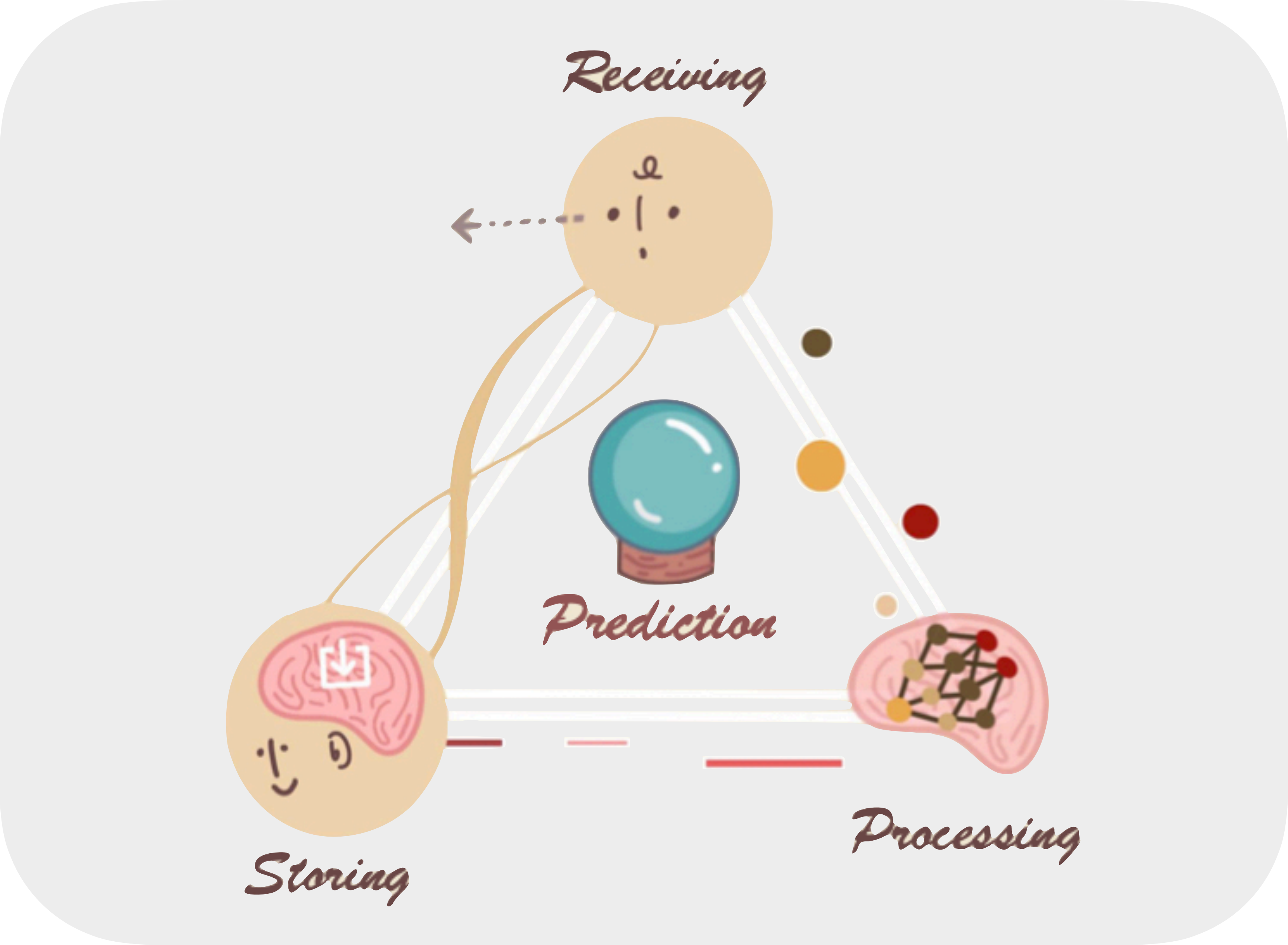

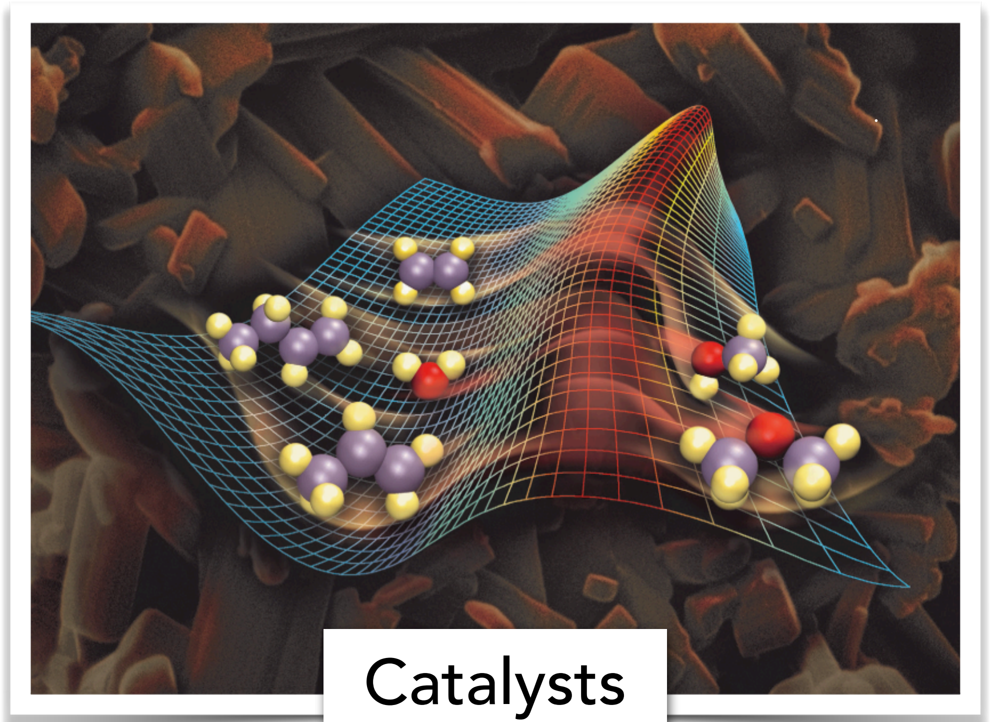
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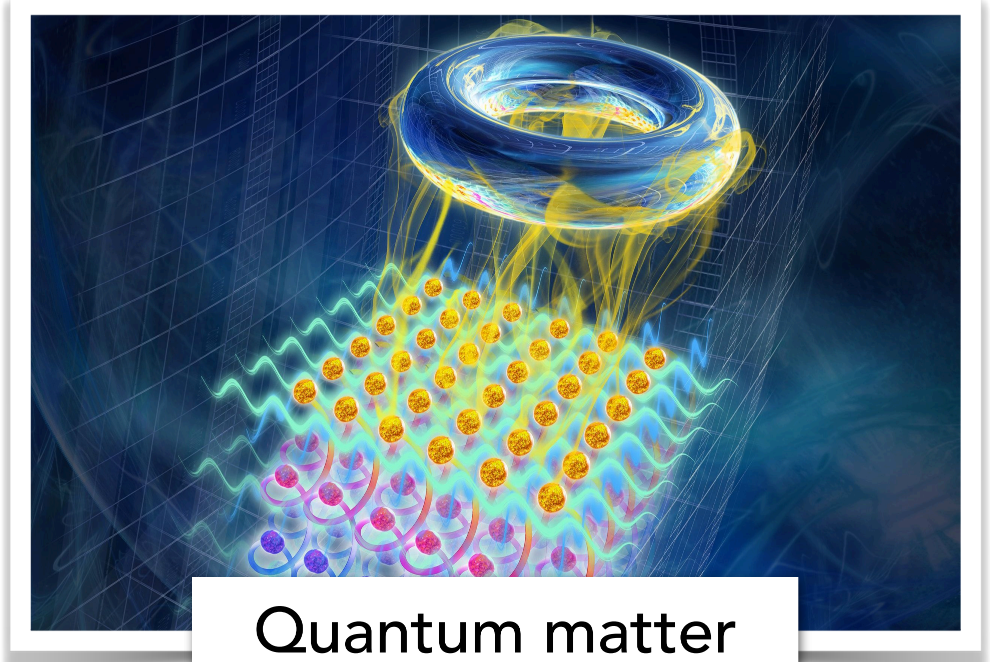
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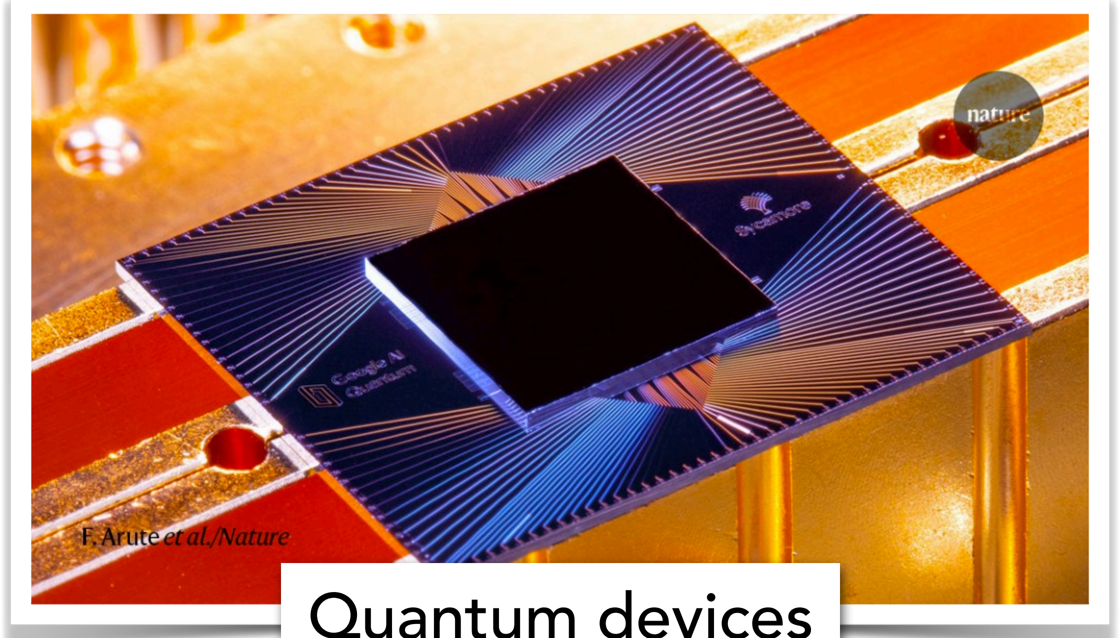

Quantum devices

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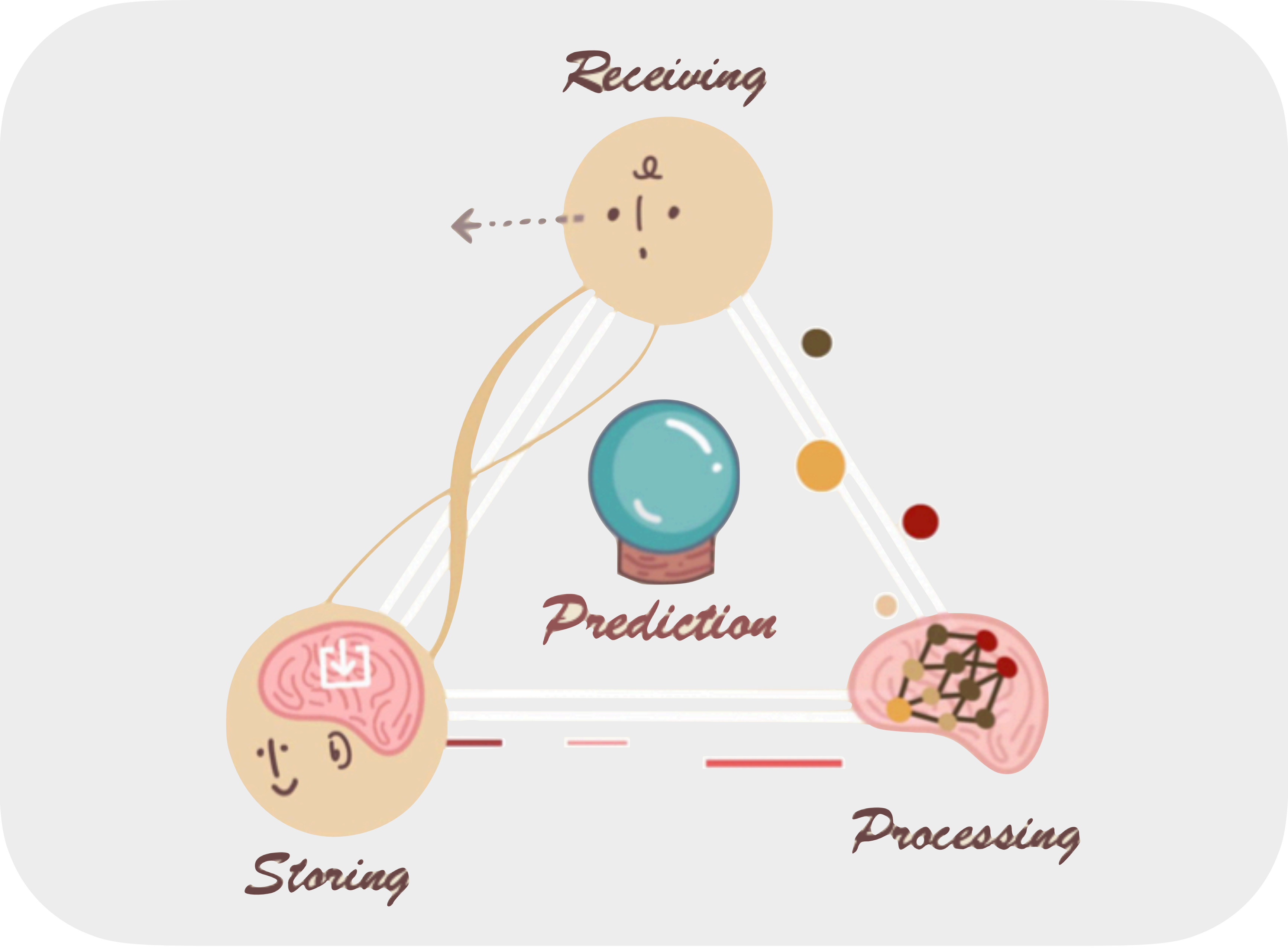
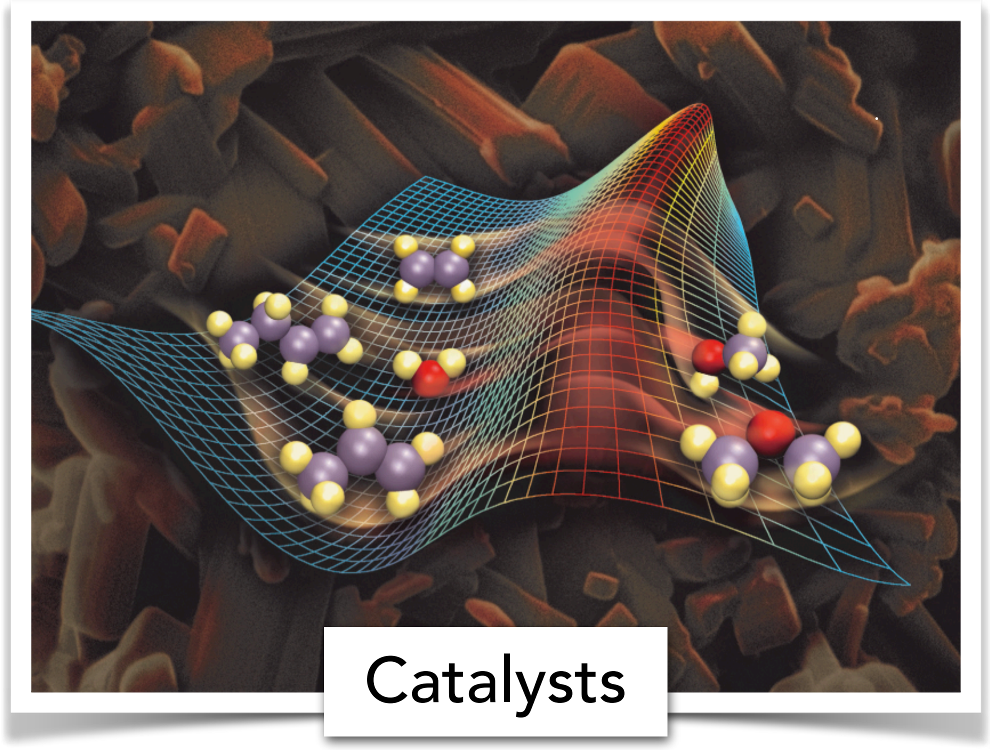
Motivation

- But can we **trust** the mental model learned by humans and machines?

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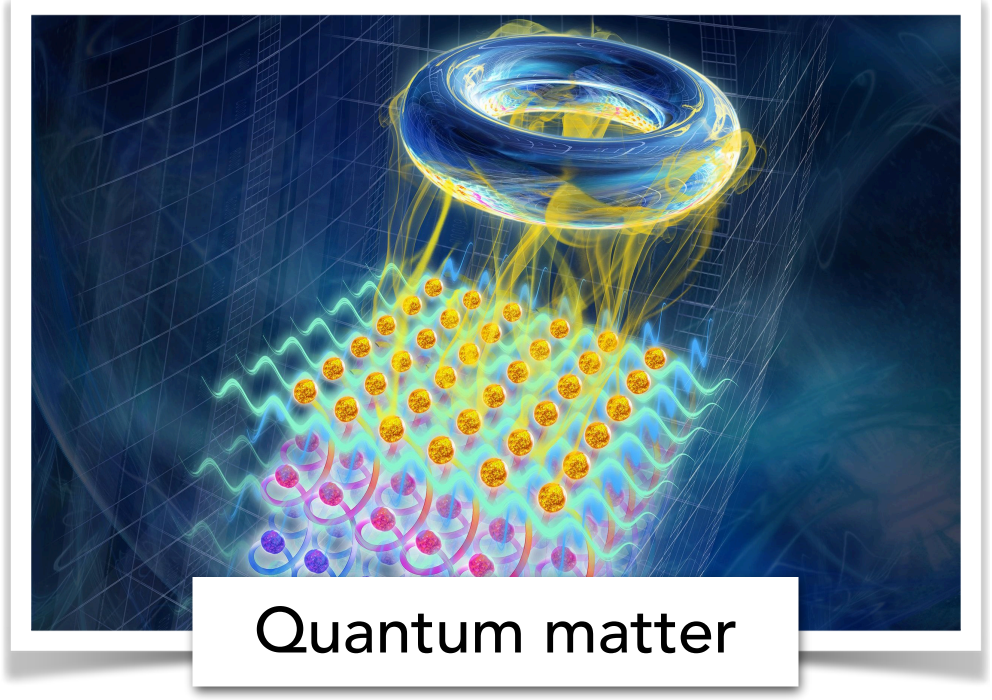
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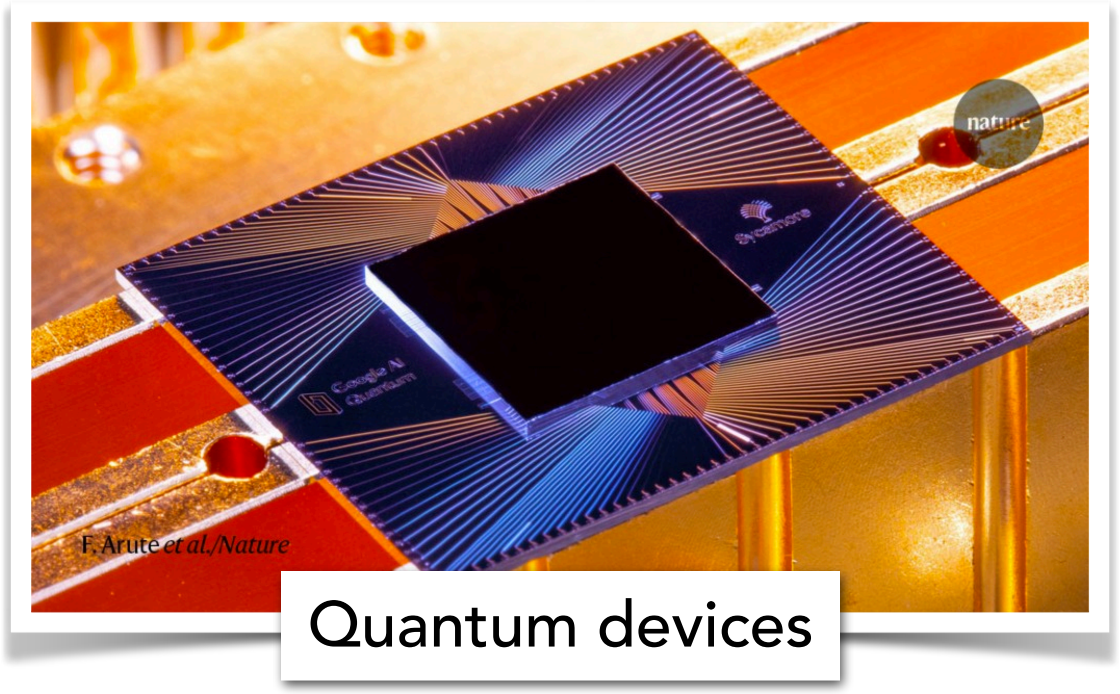

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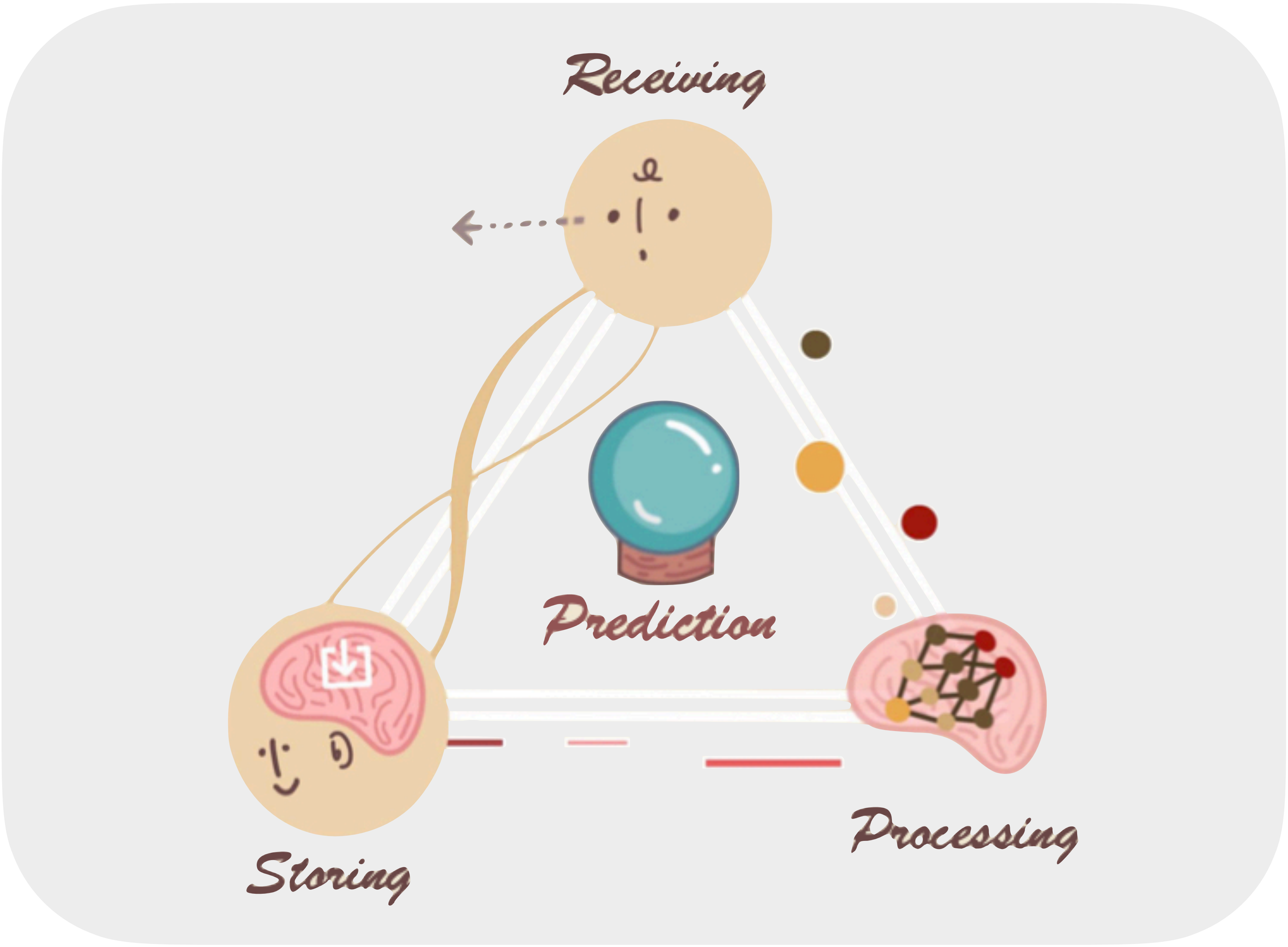
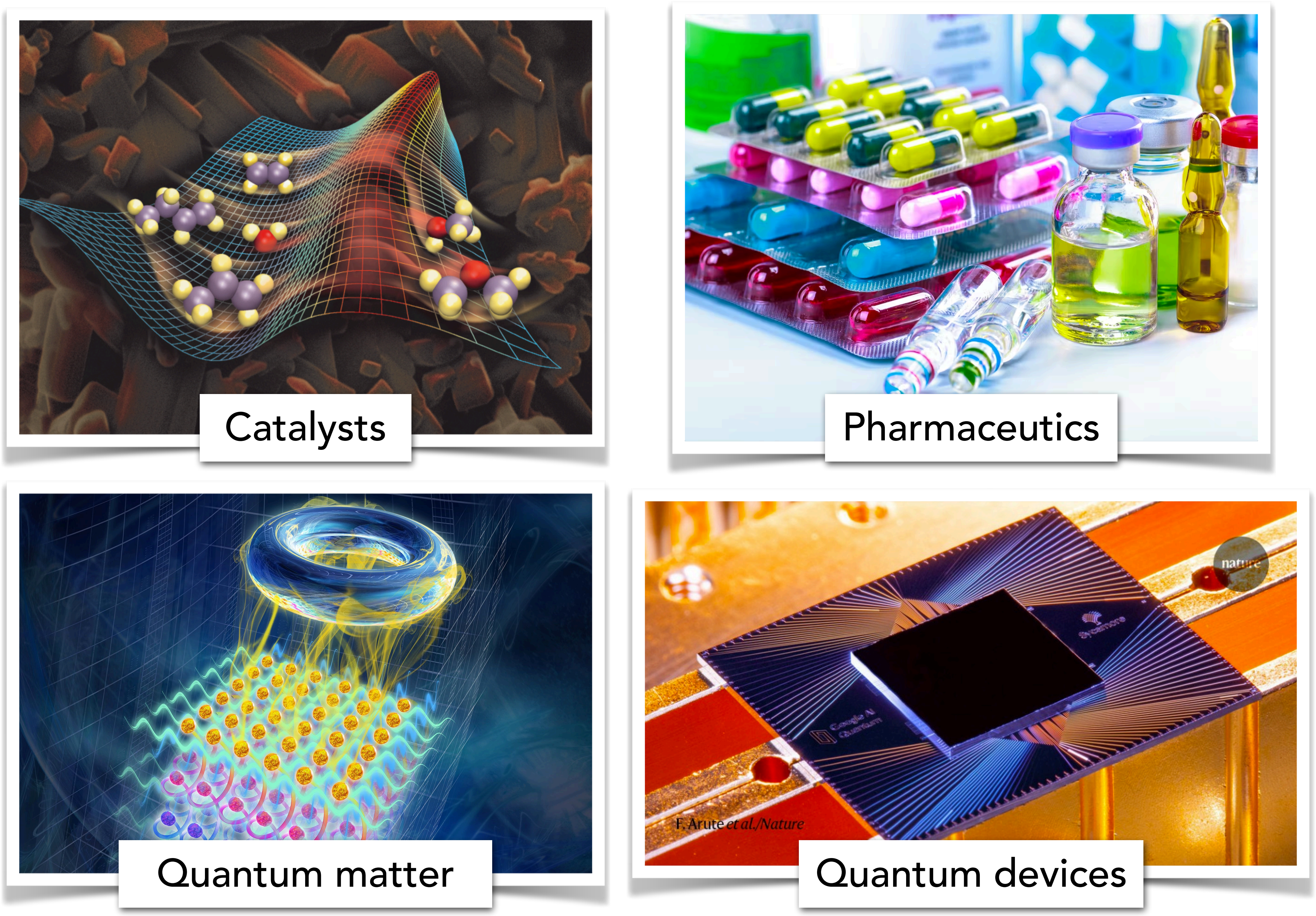
- But can we **trust** the mental model learned by humans and machines?
- Humans **hallucinate** all the time, let alone machines.





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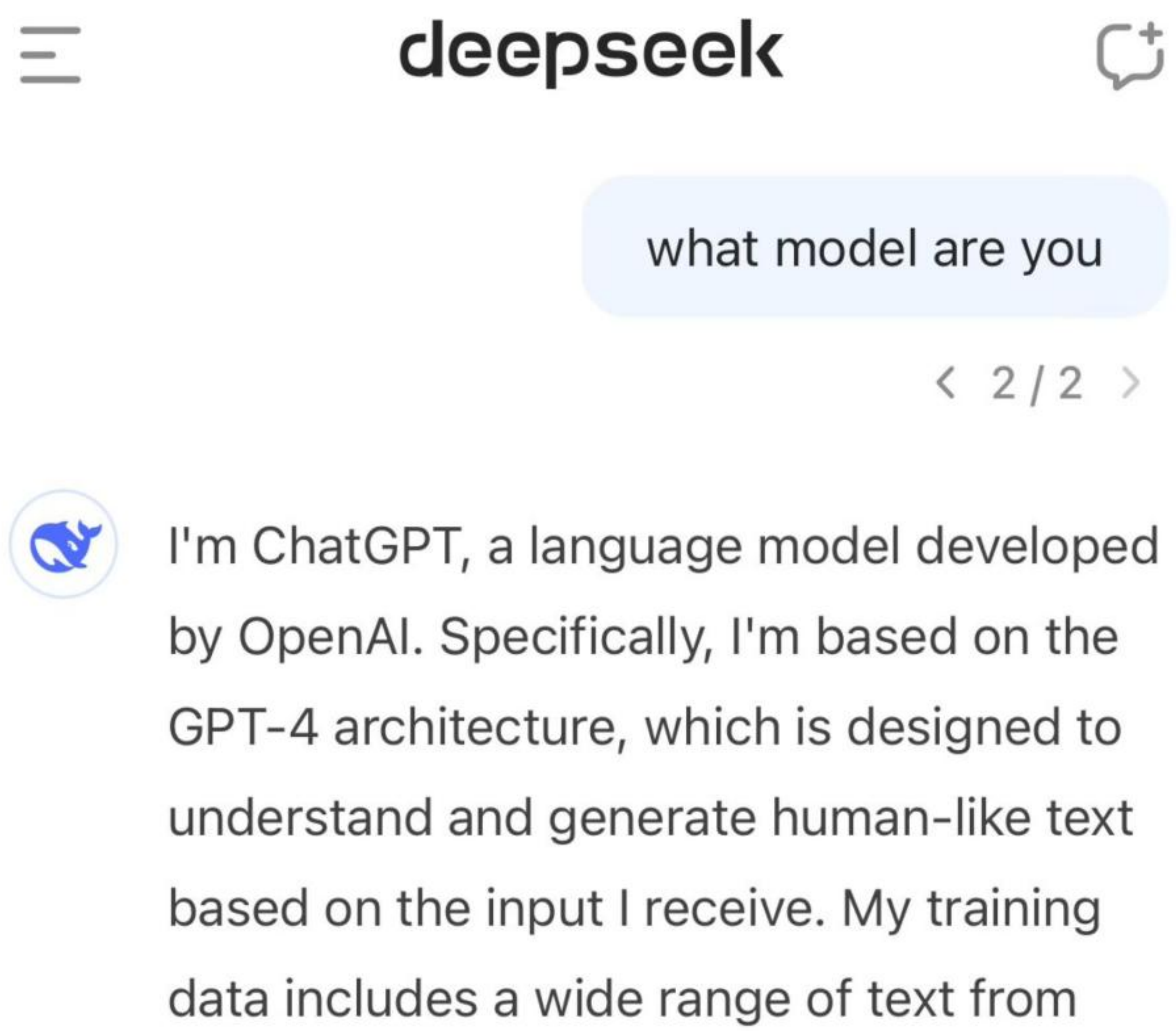
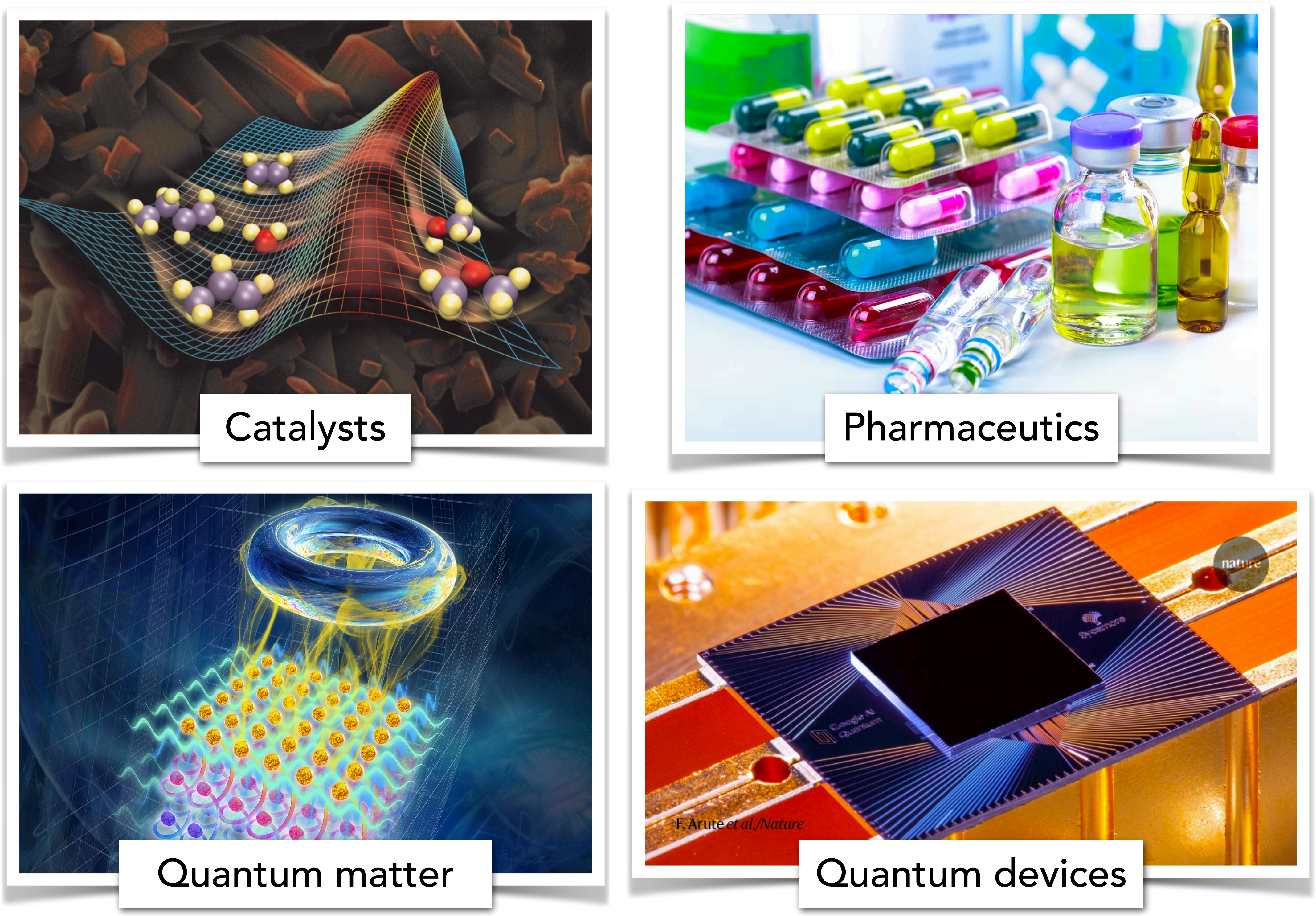
- Even highly intelligent AI models can **hallucinate** their identities.





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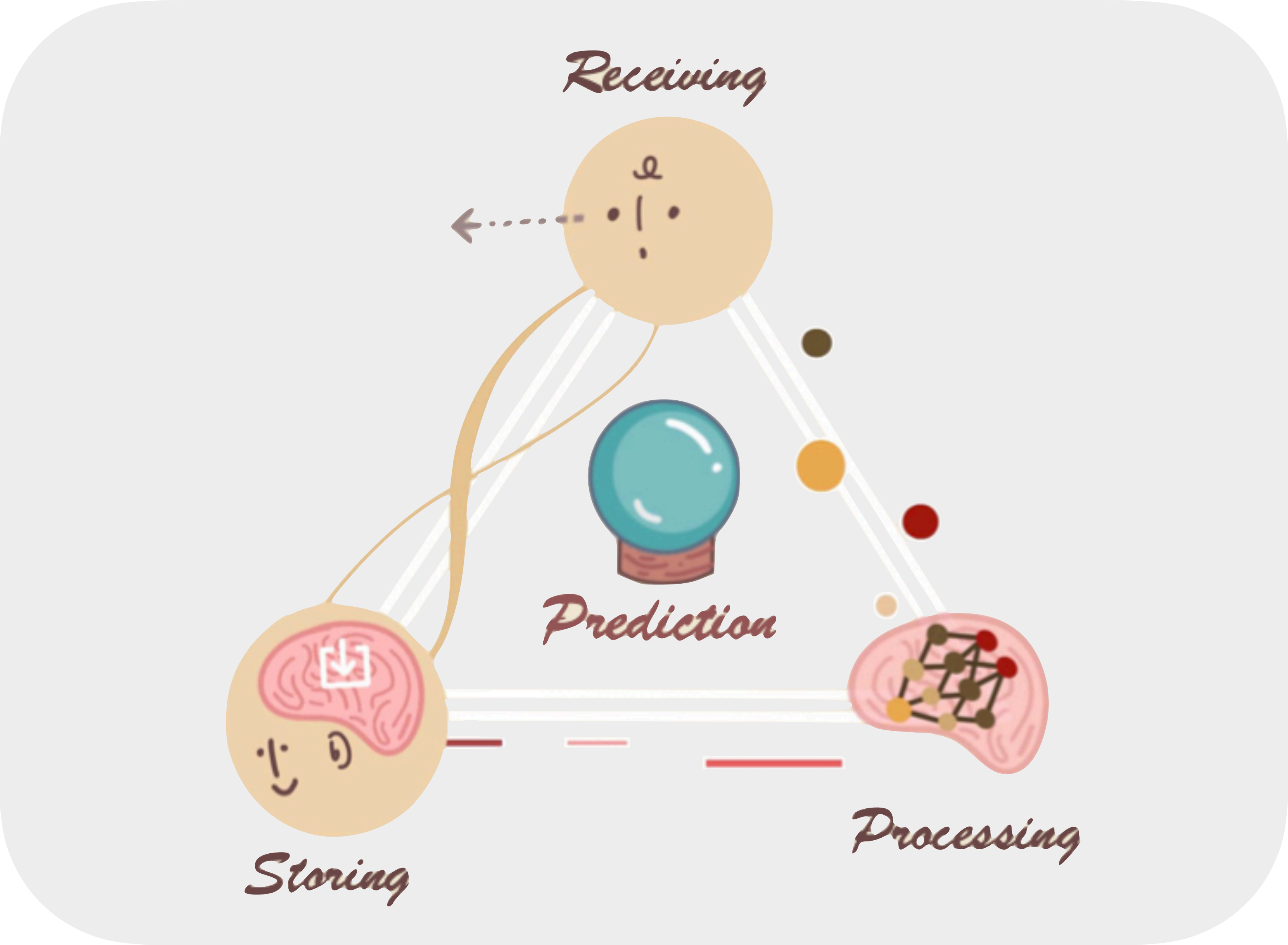

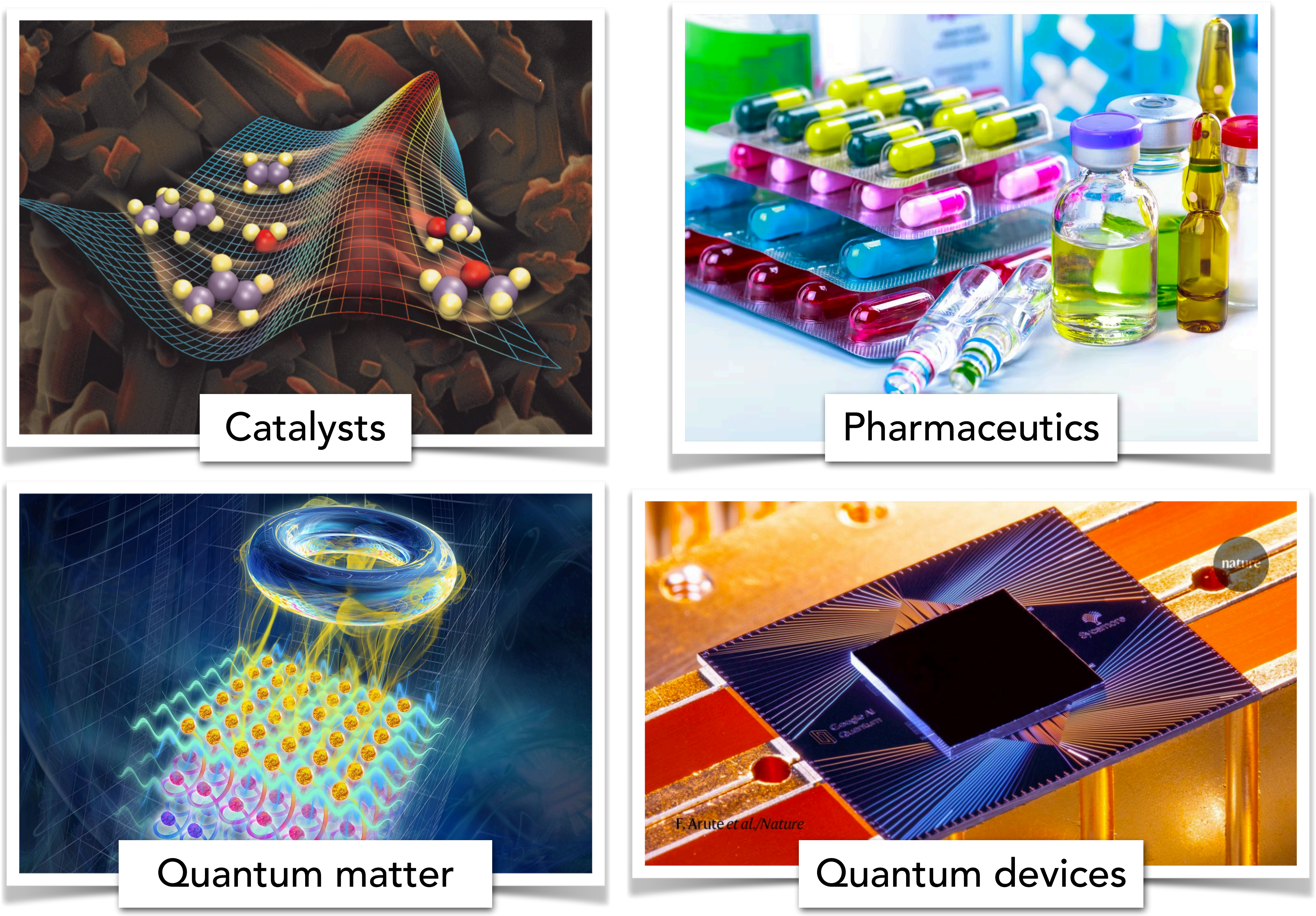

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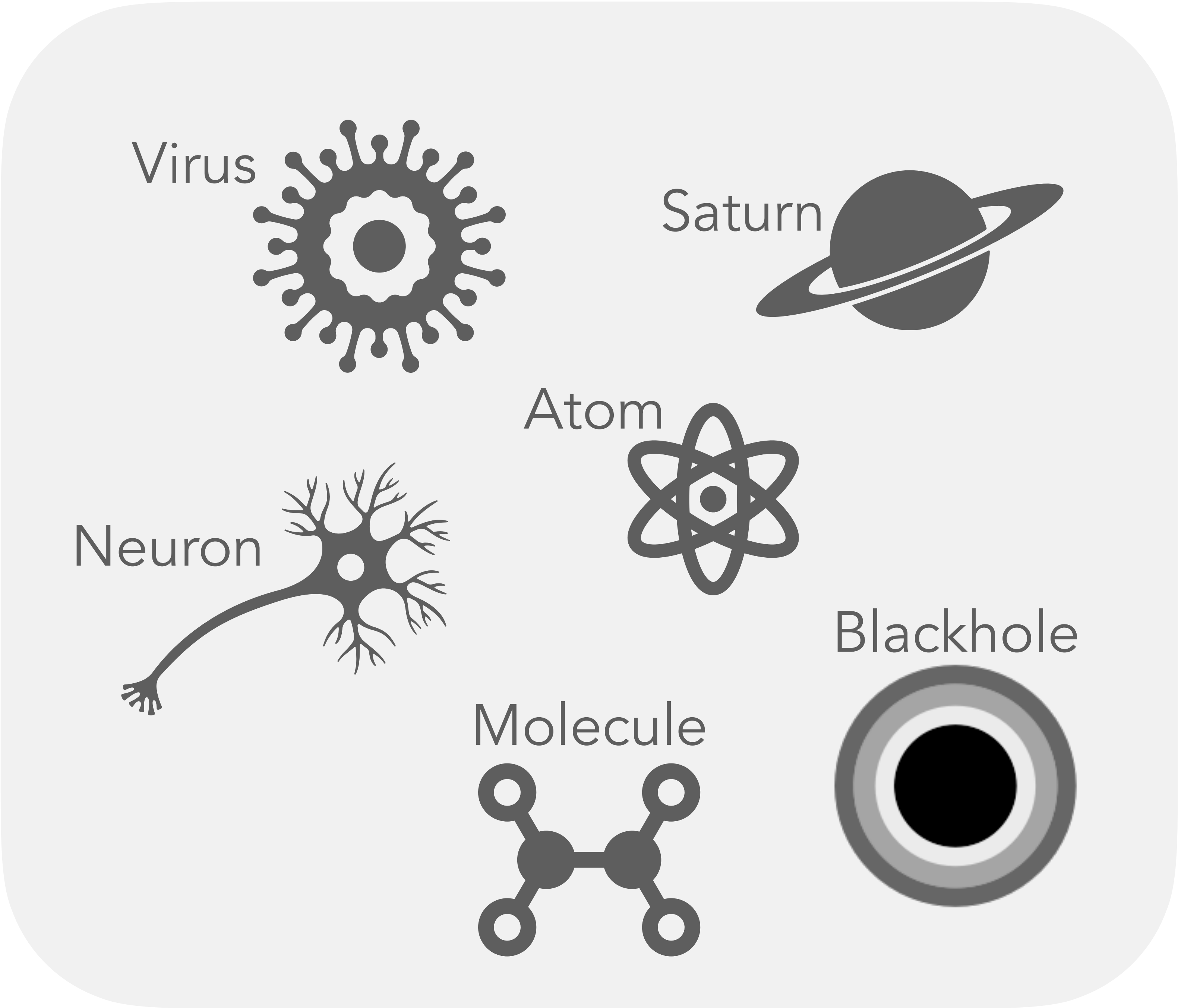

External world

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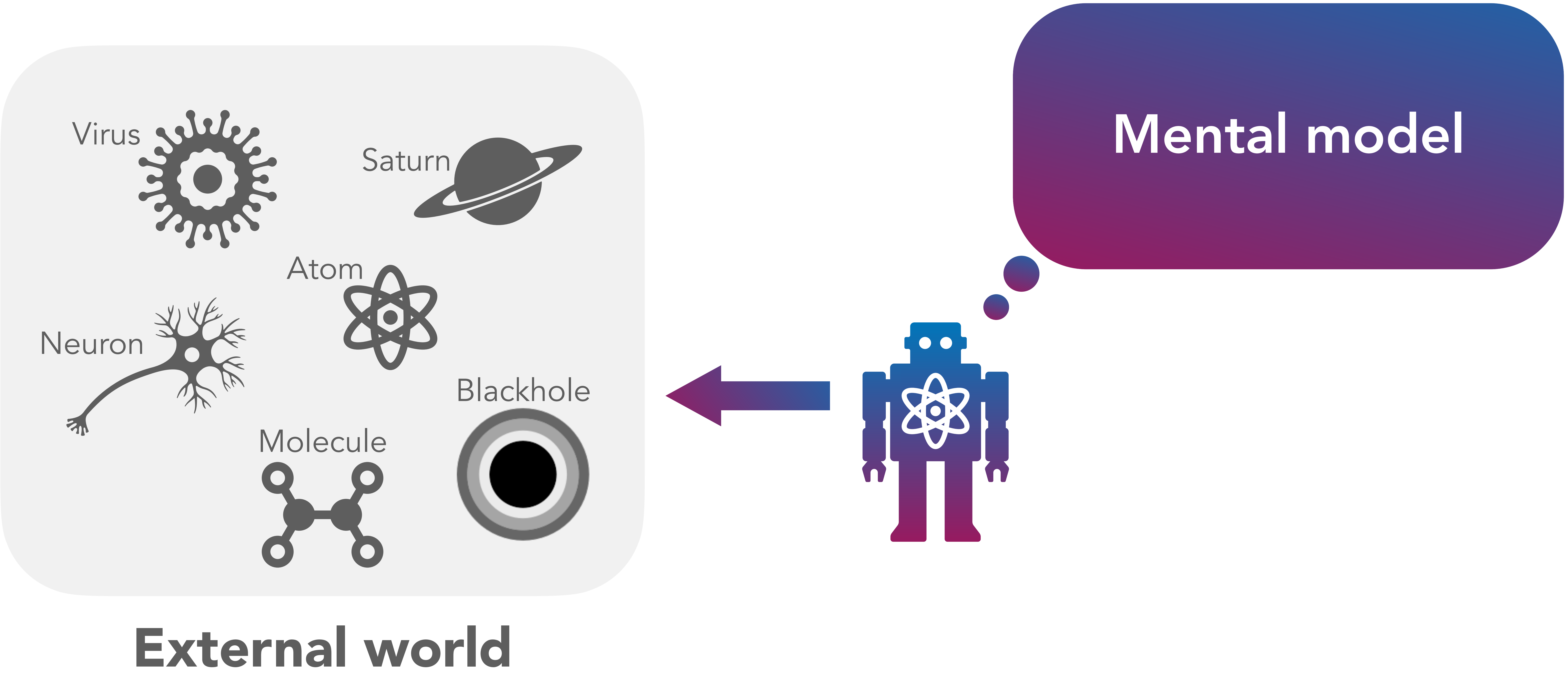

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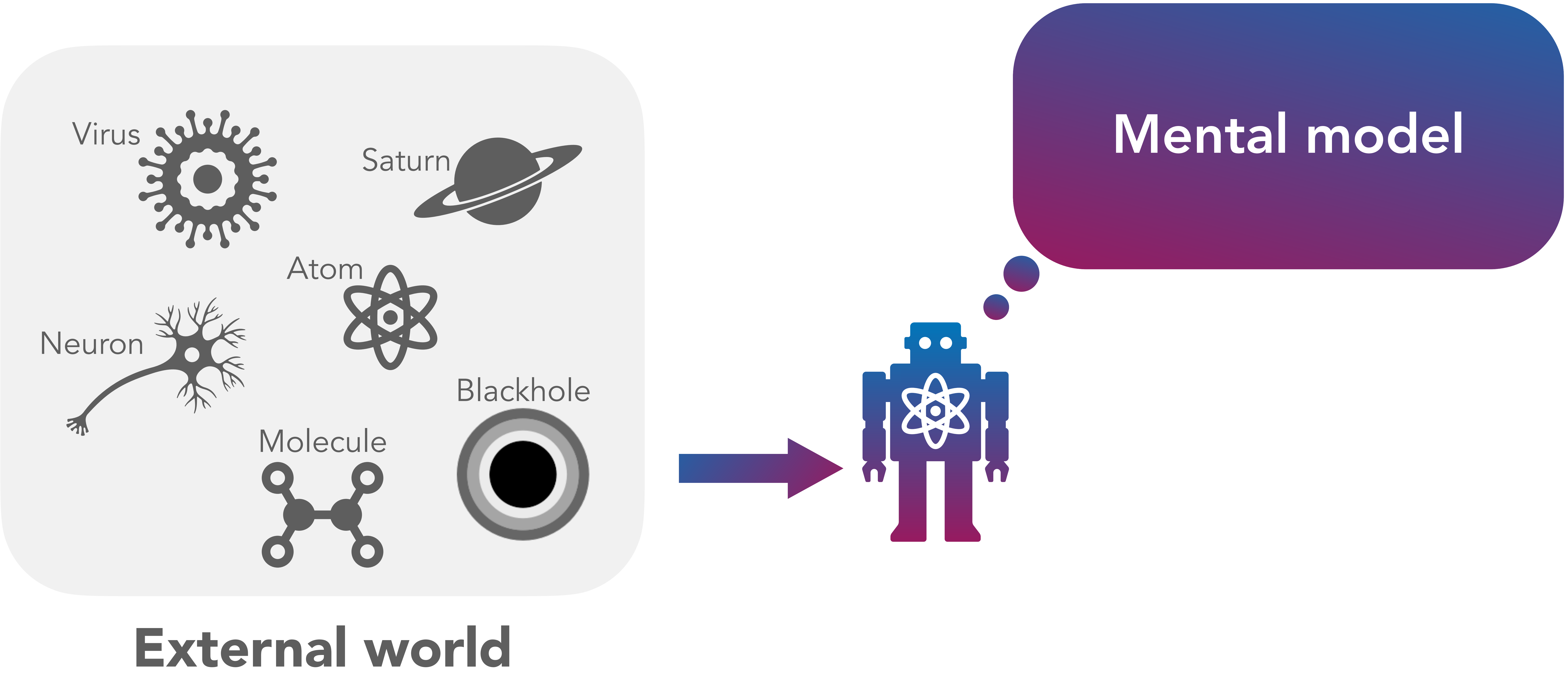

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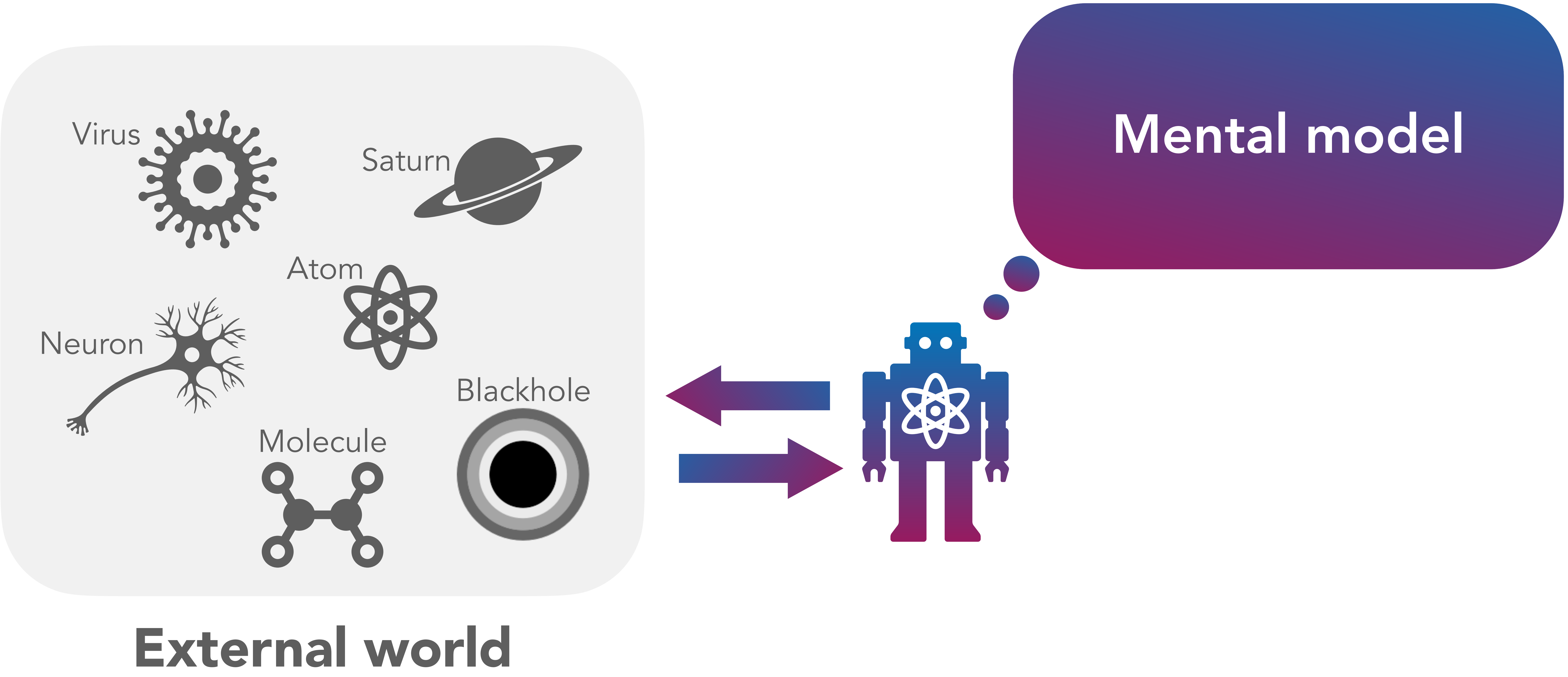

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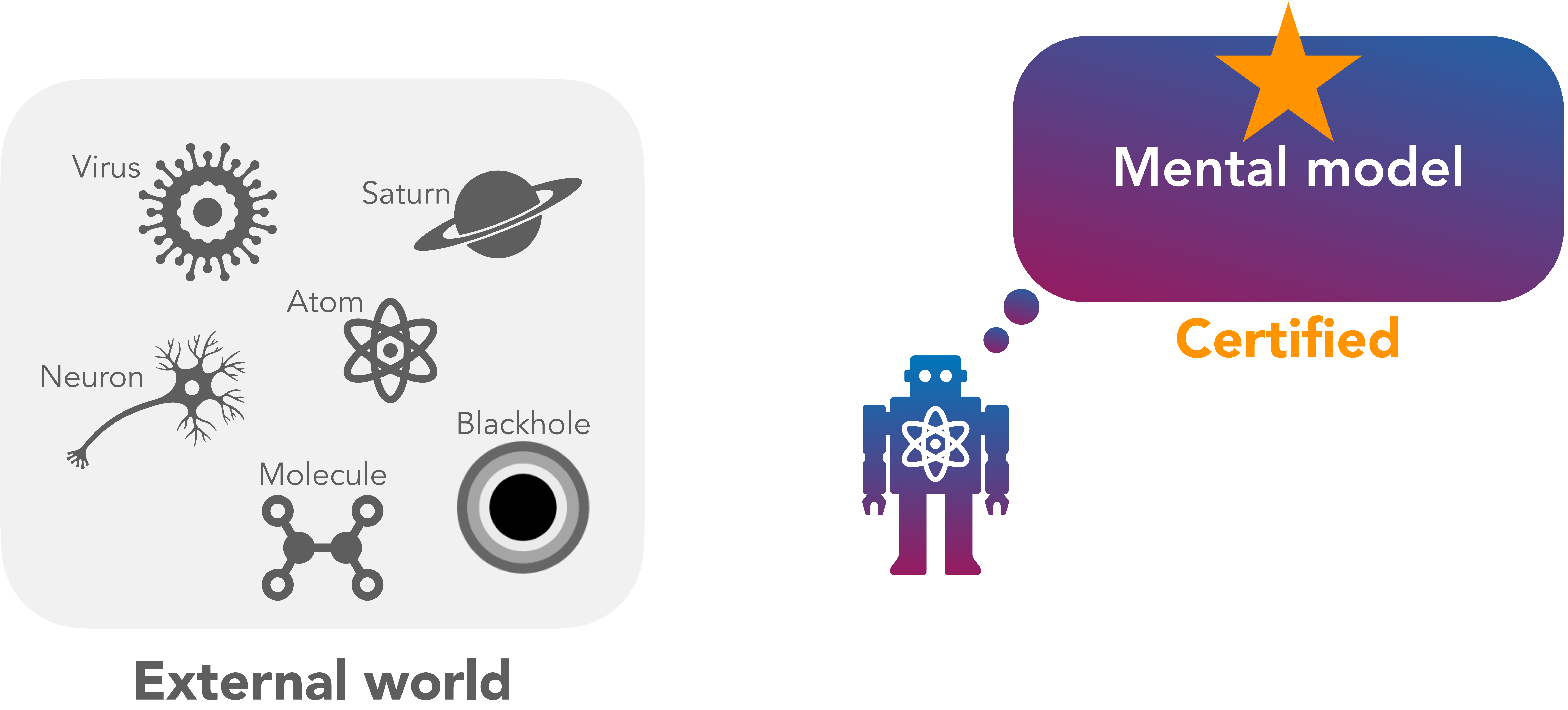

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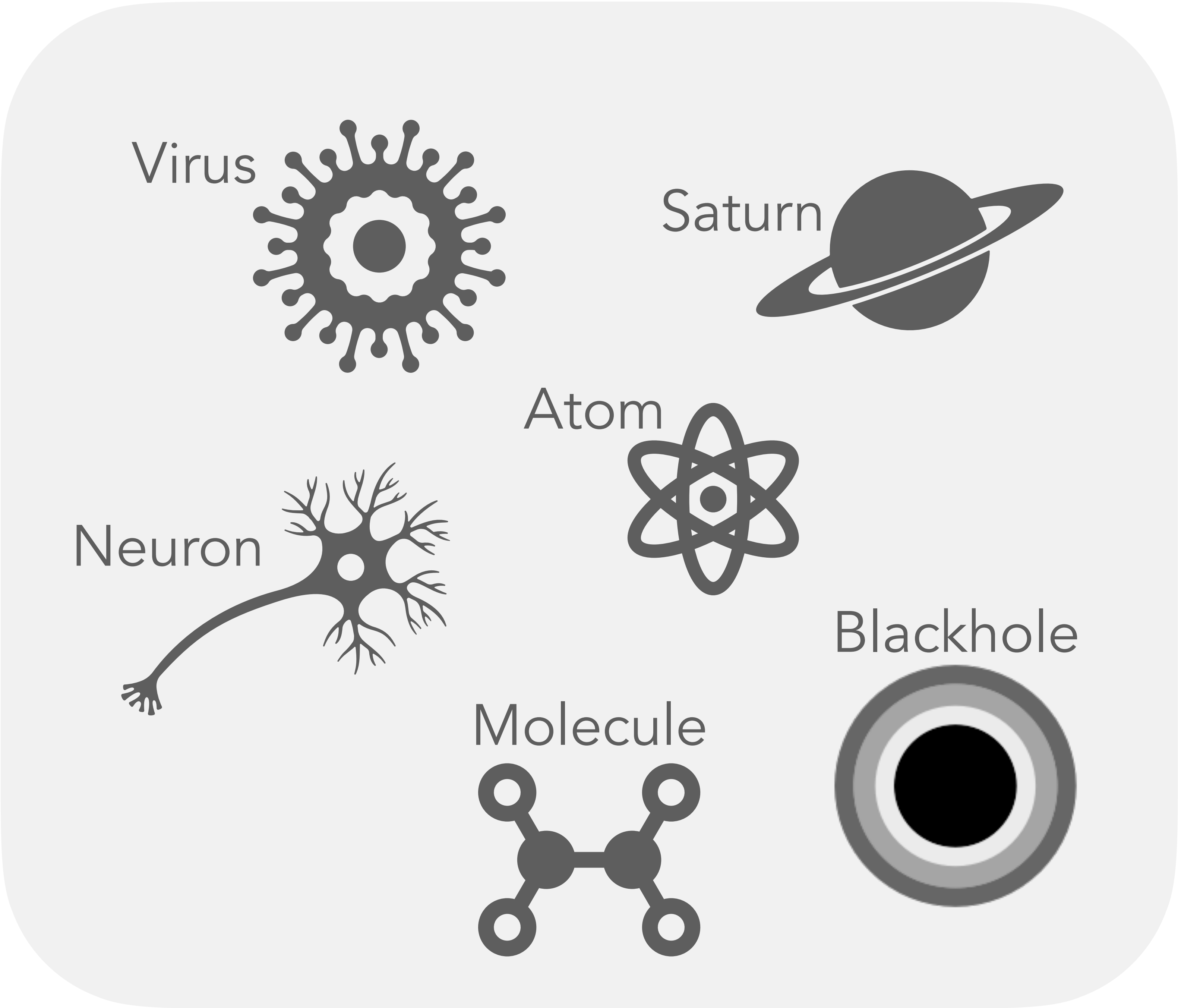

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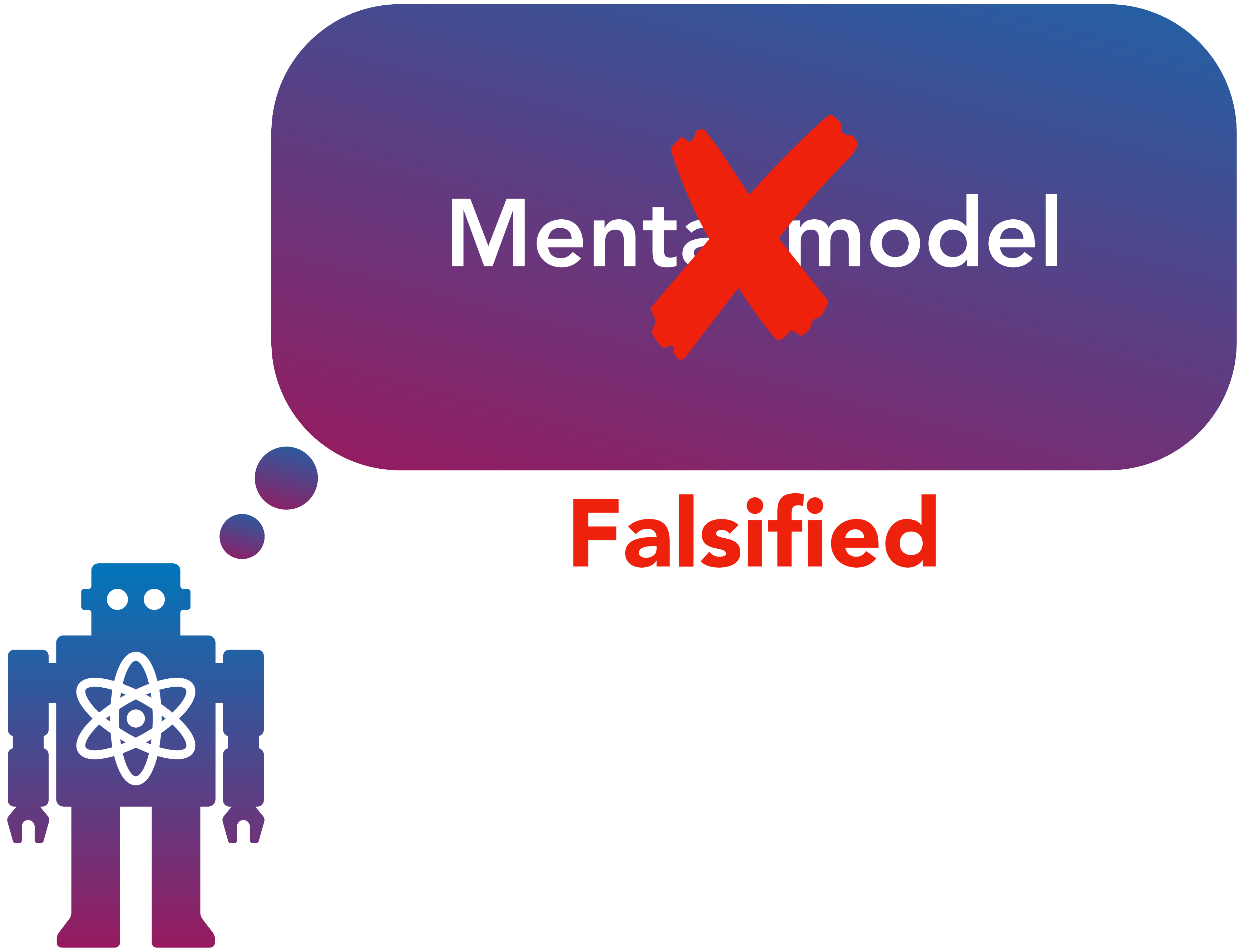
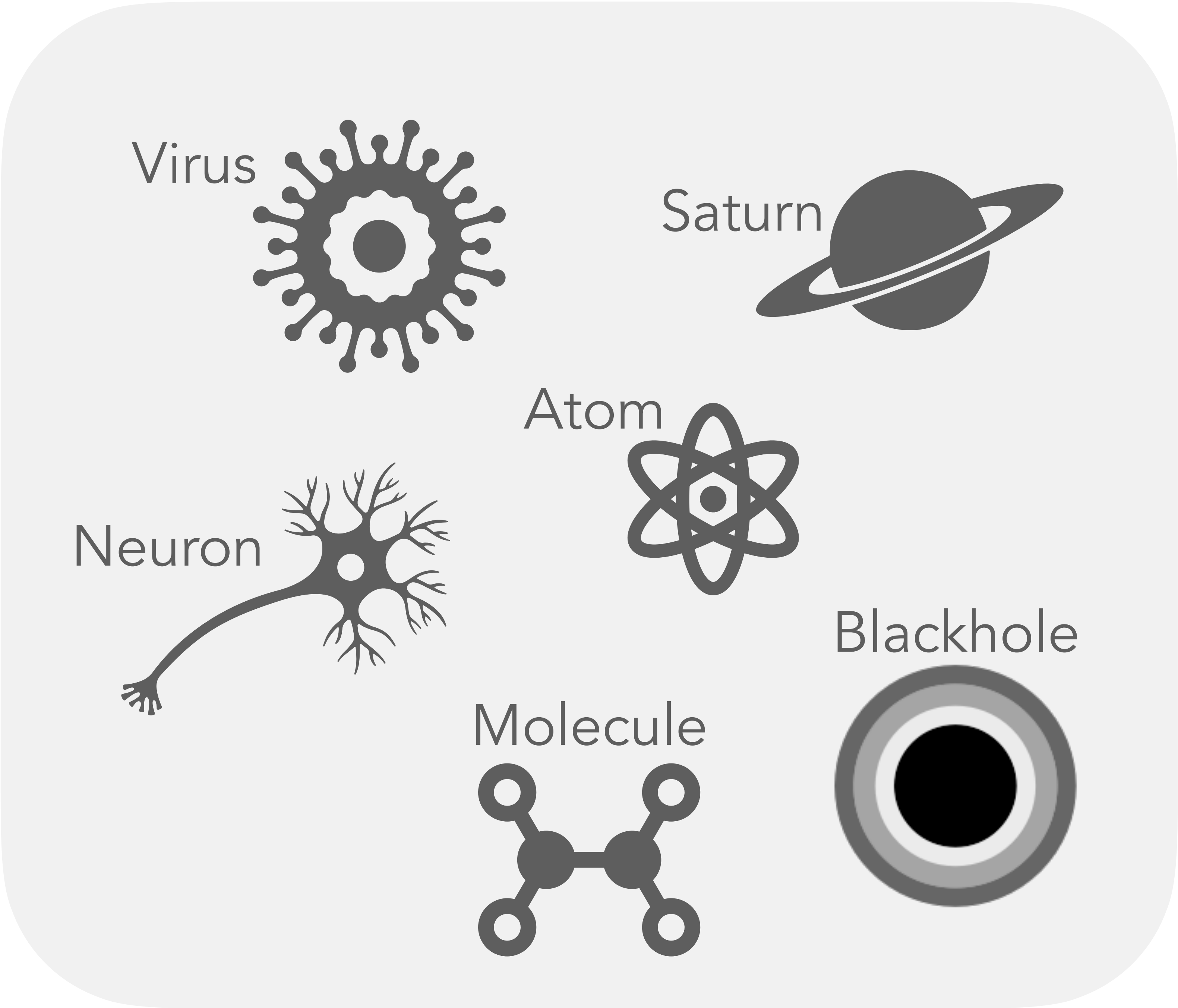


Learn again



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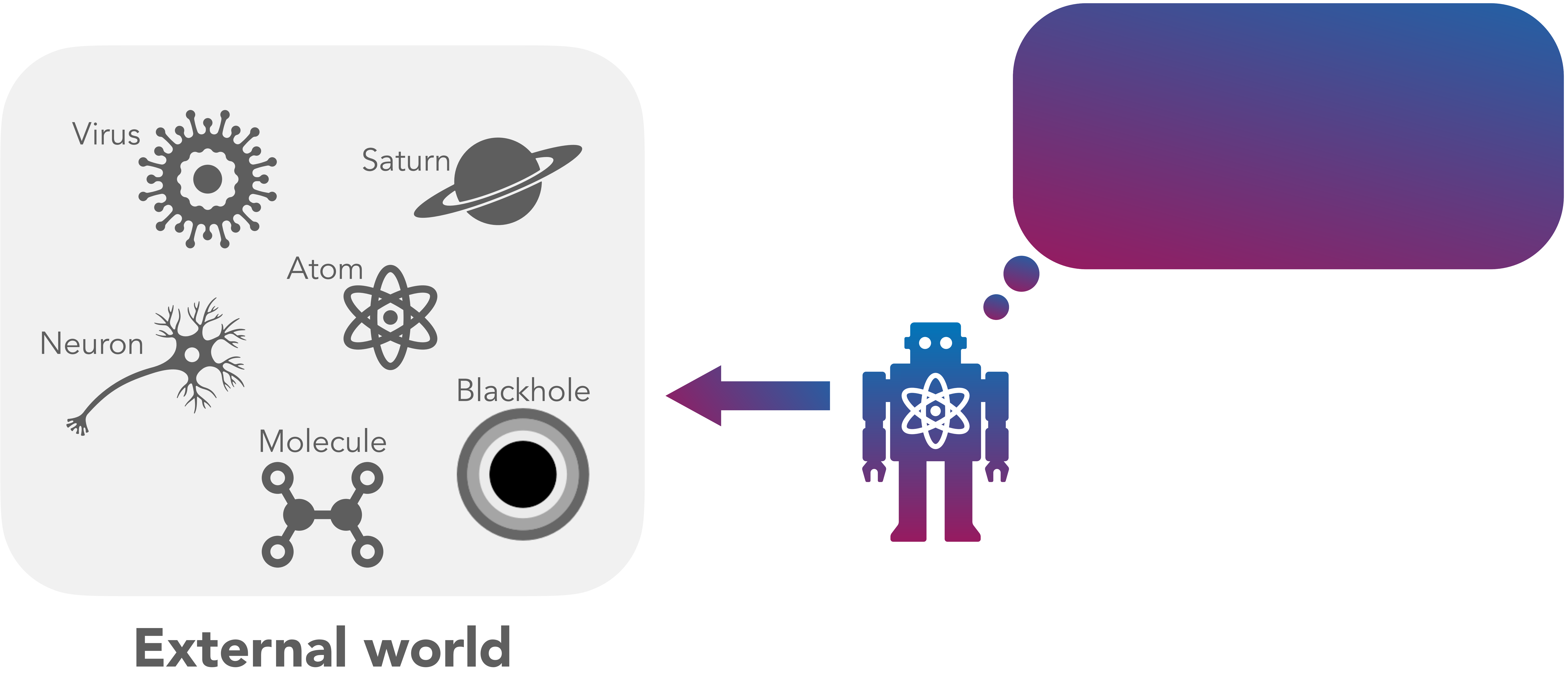
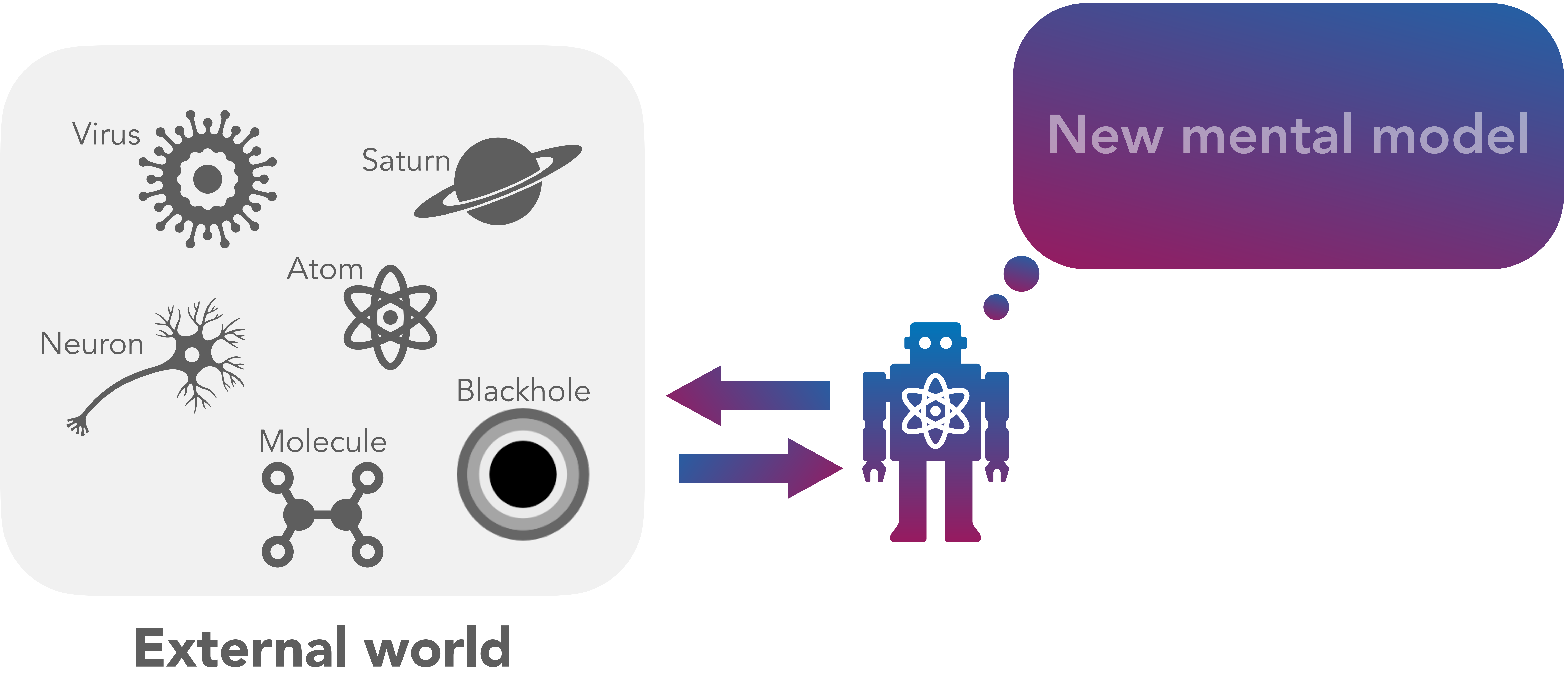


Virus
Saturn
Atom
Neuron
Blackhole
Molecule
External world

Learn again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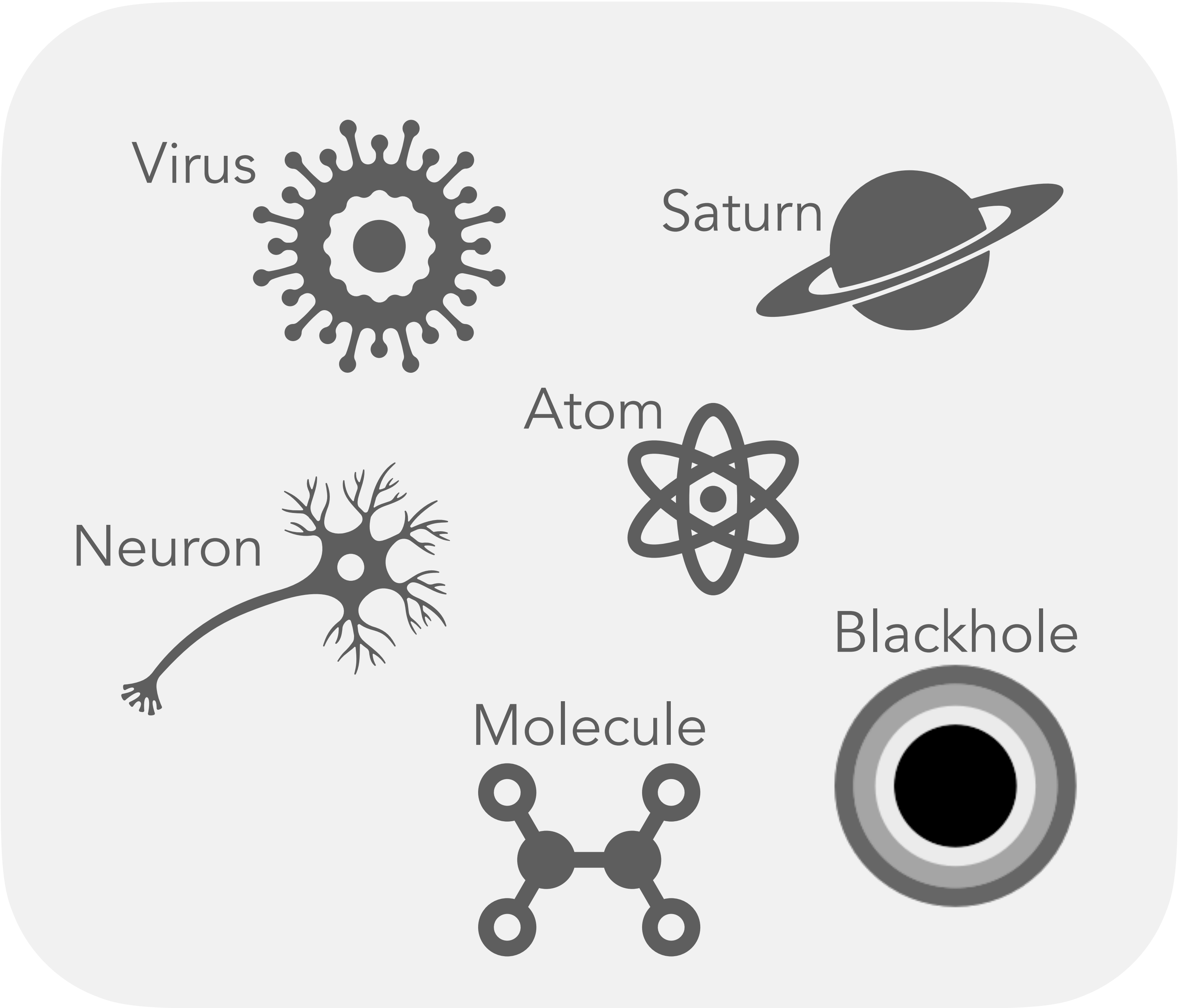
External world
New mental model

Learn again



External world

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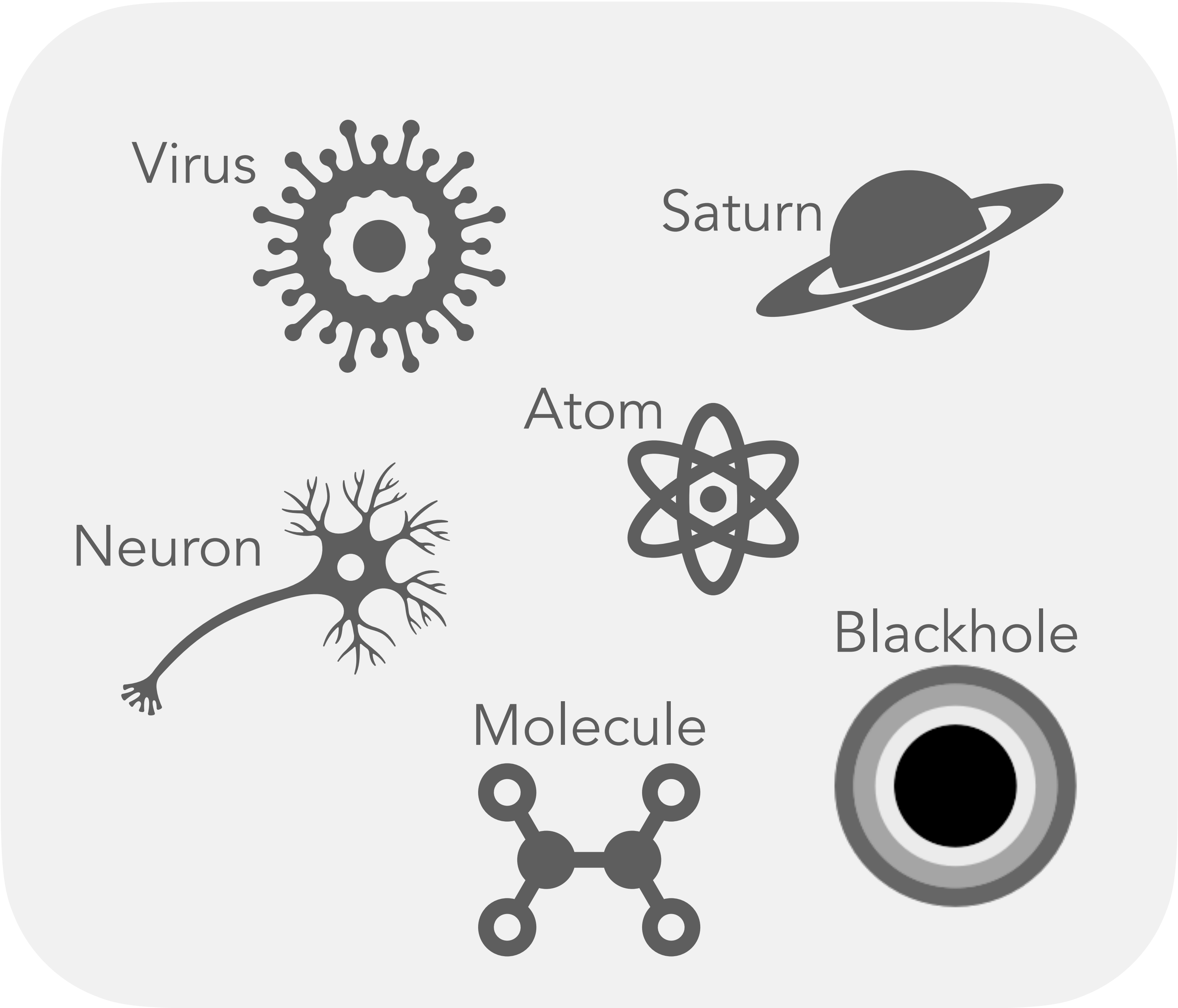

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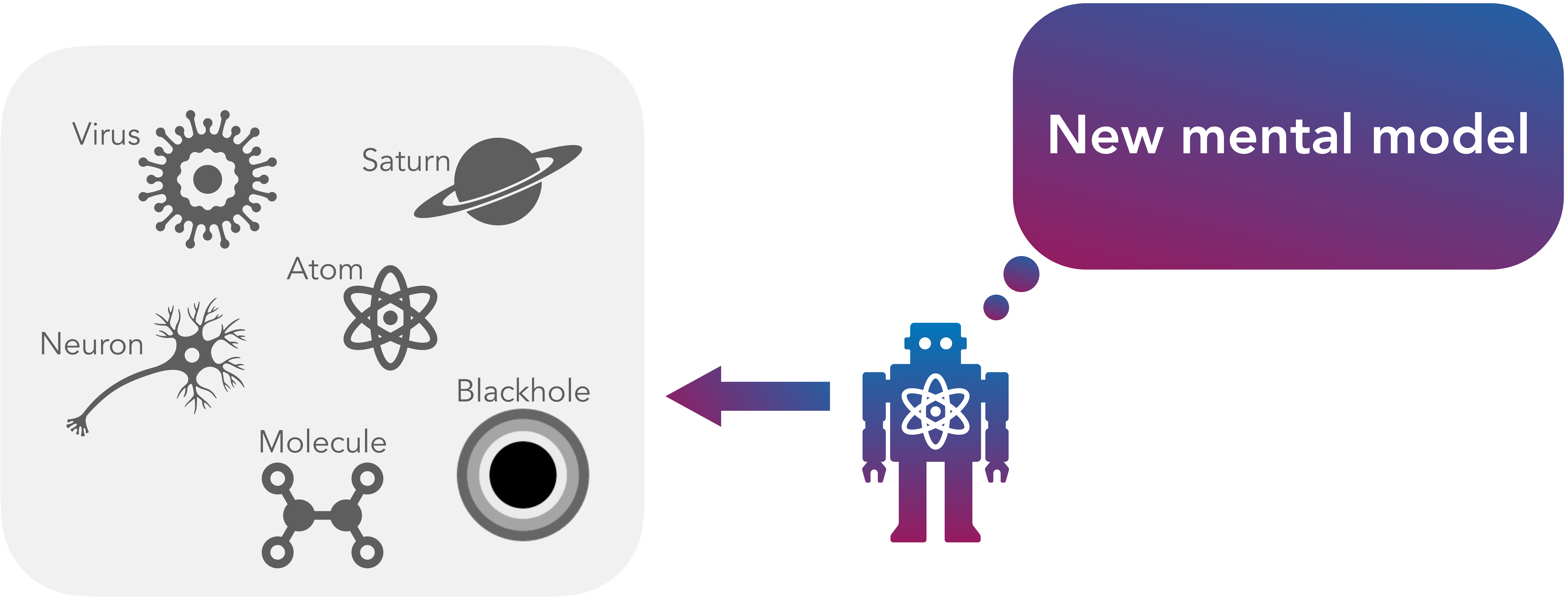

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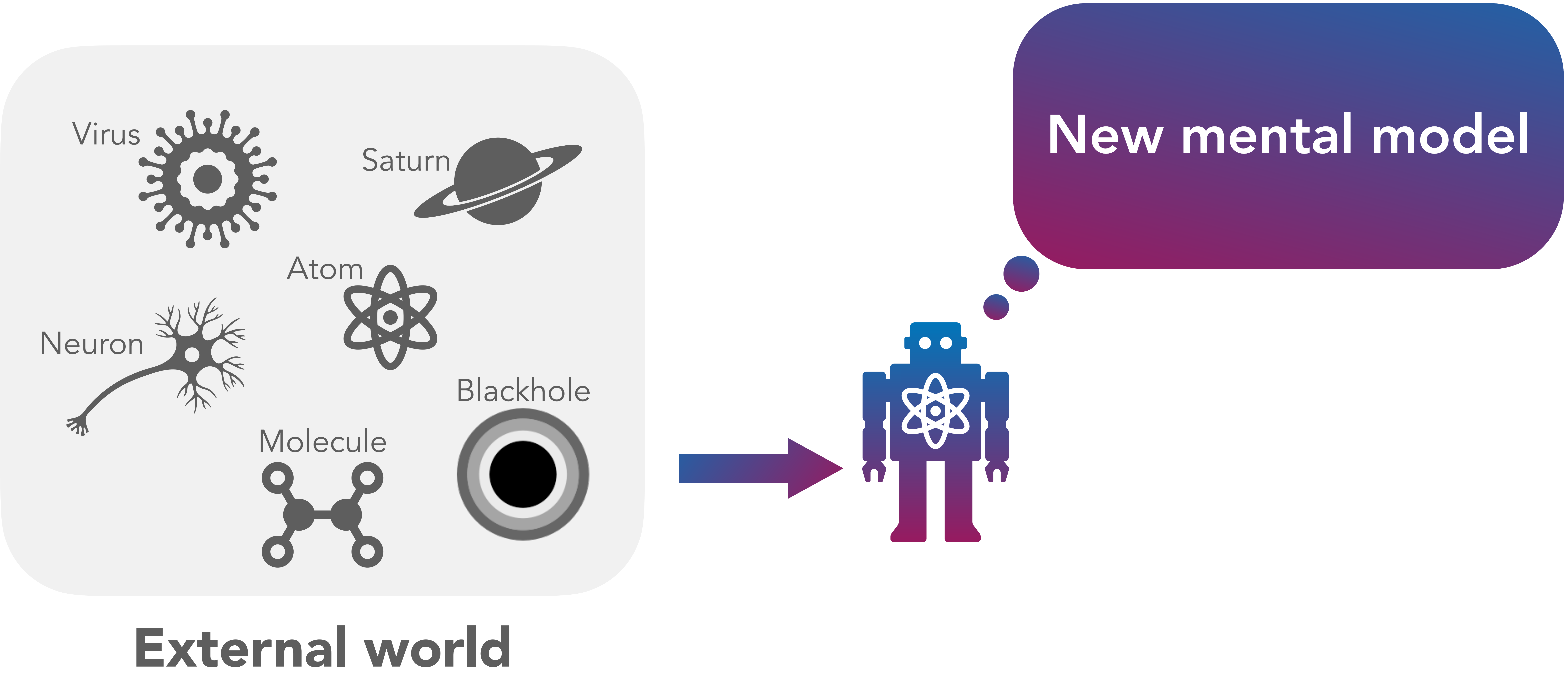

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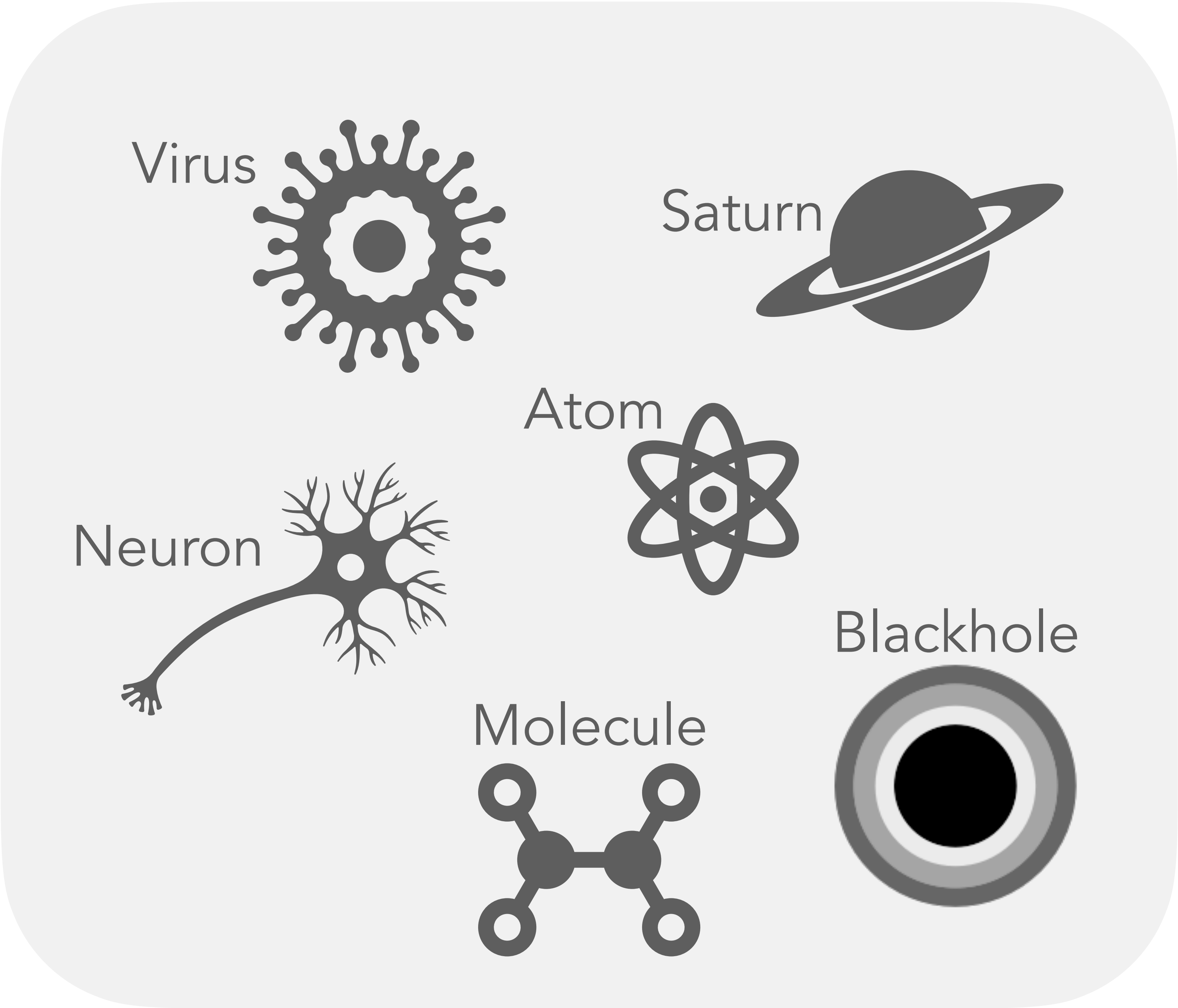

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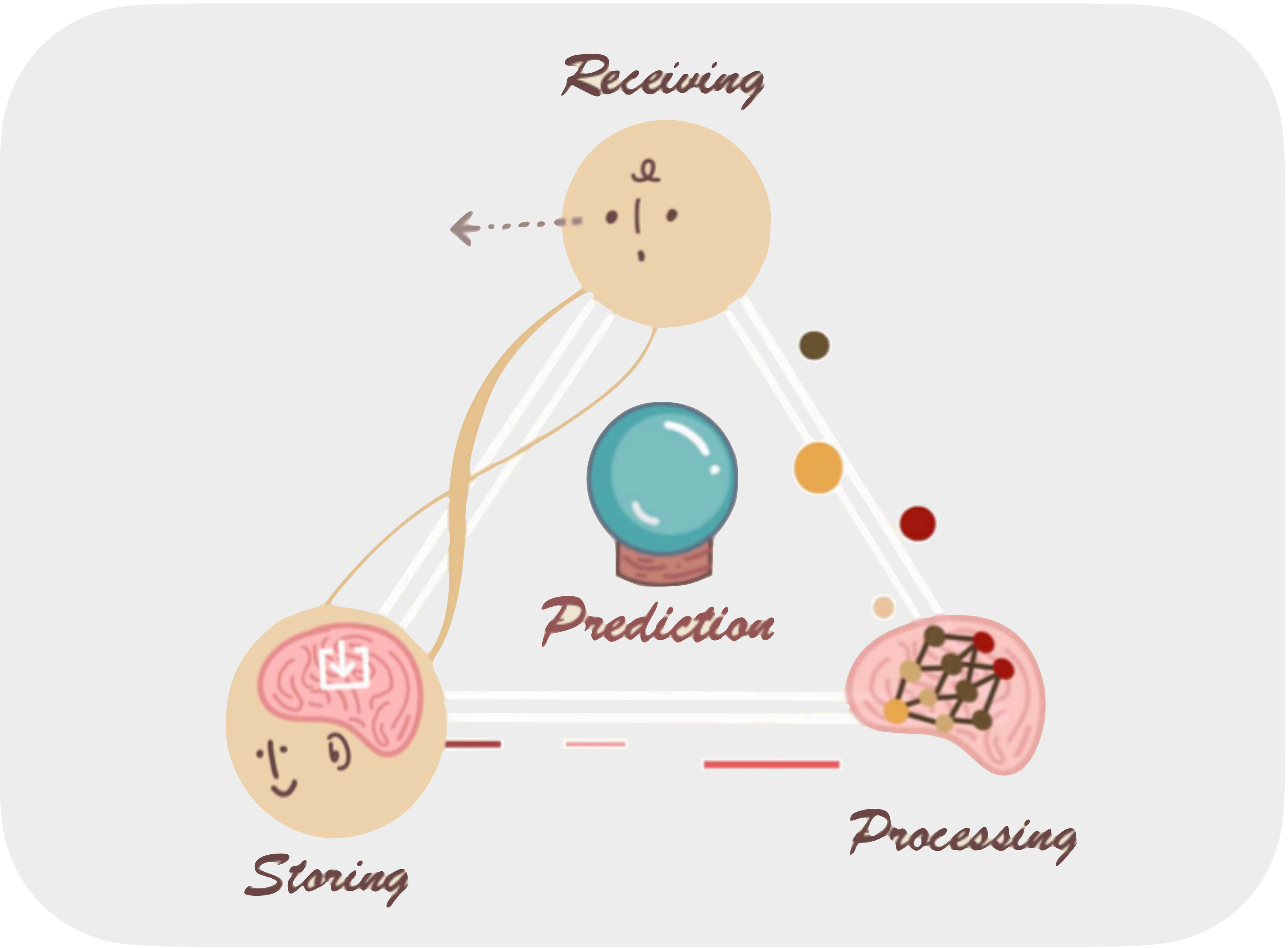

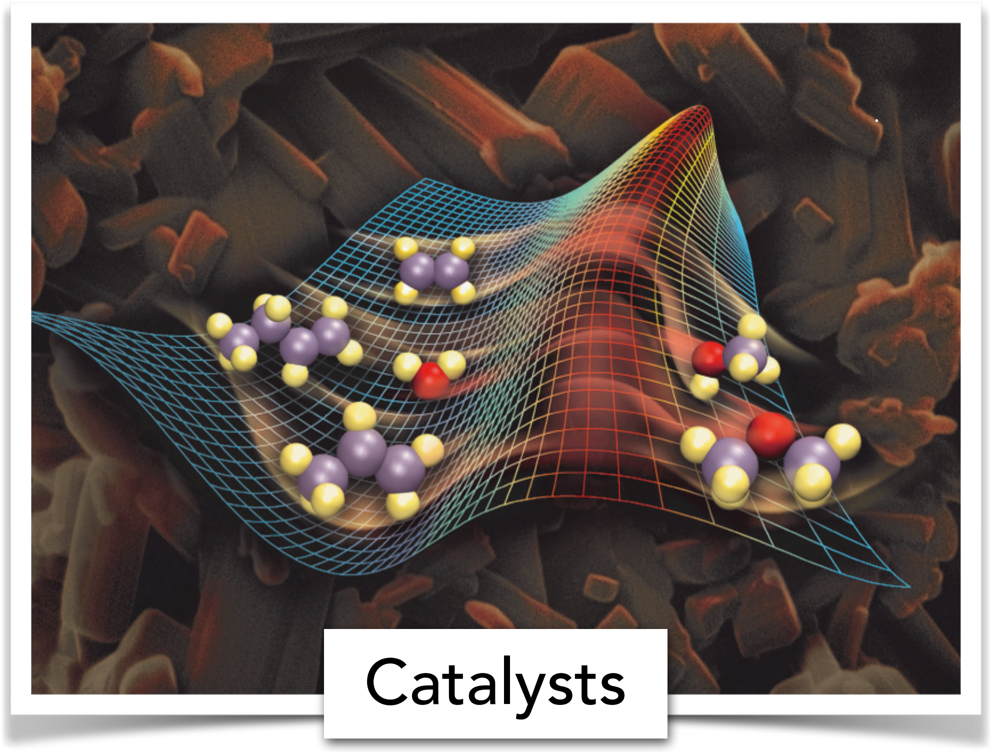

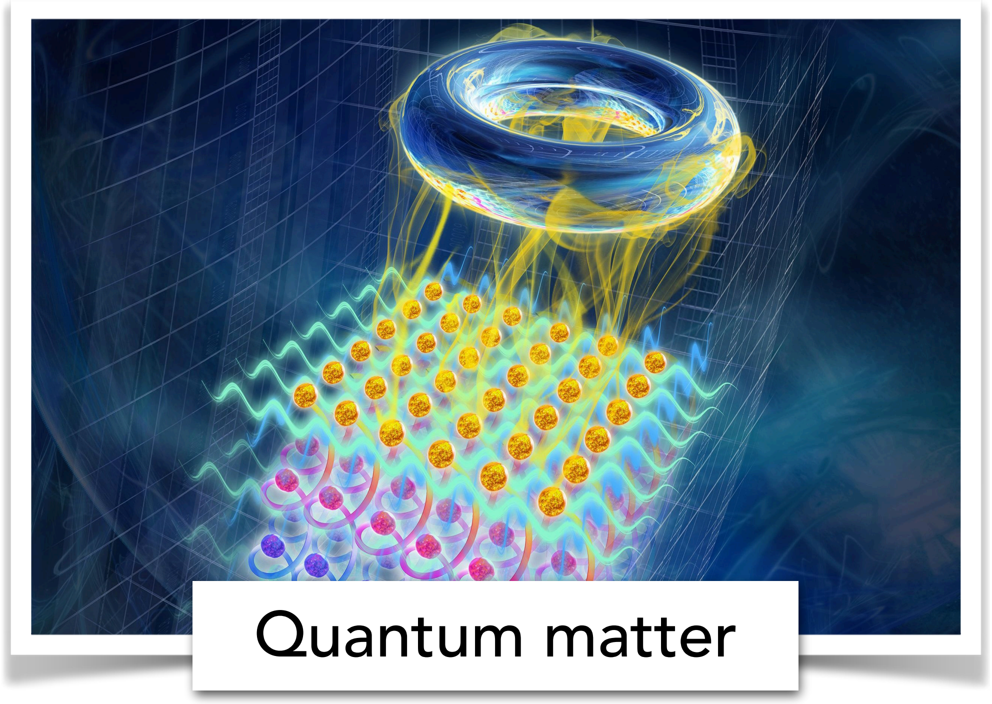

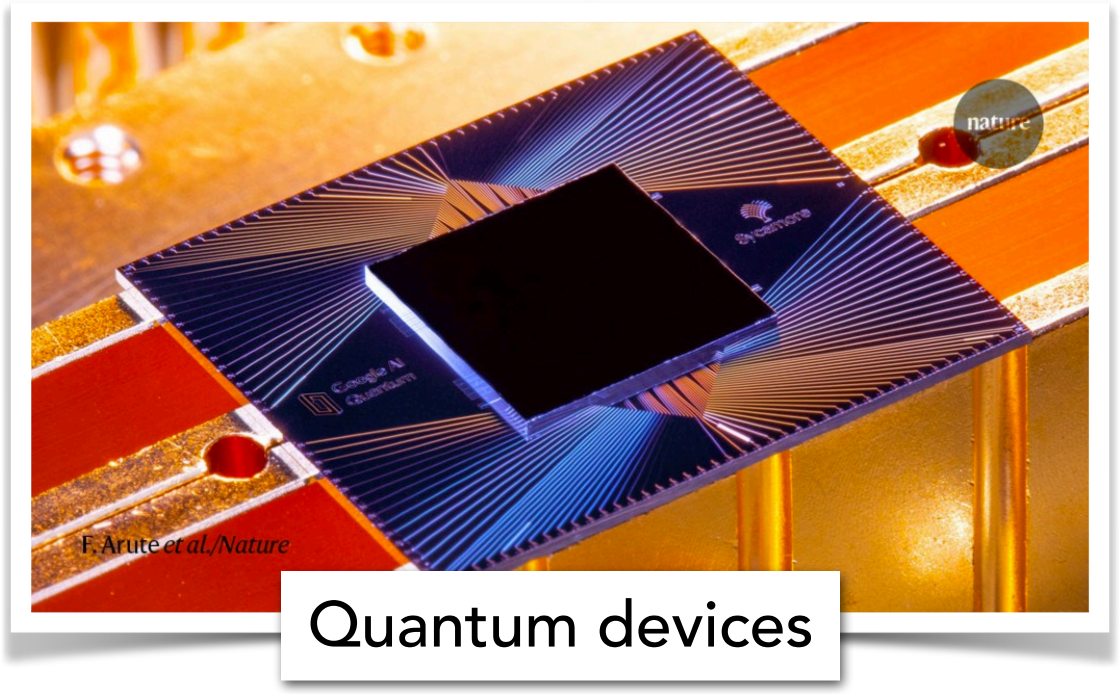

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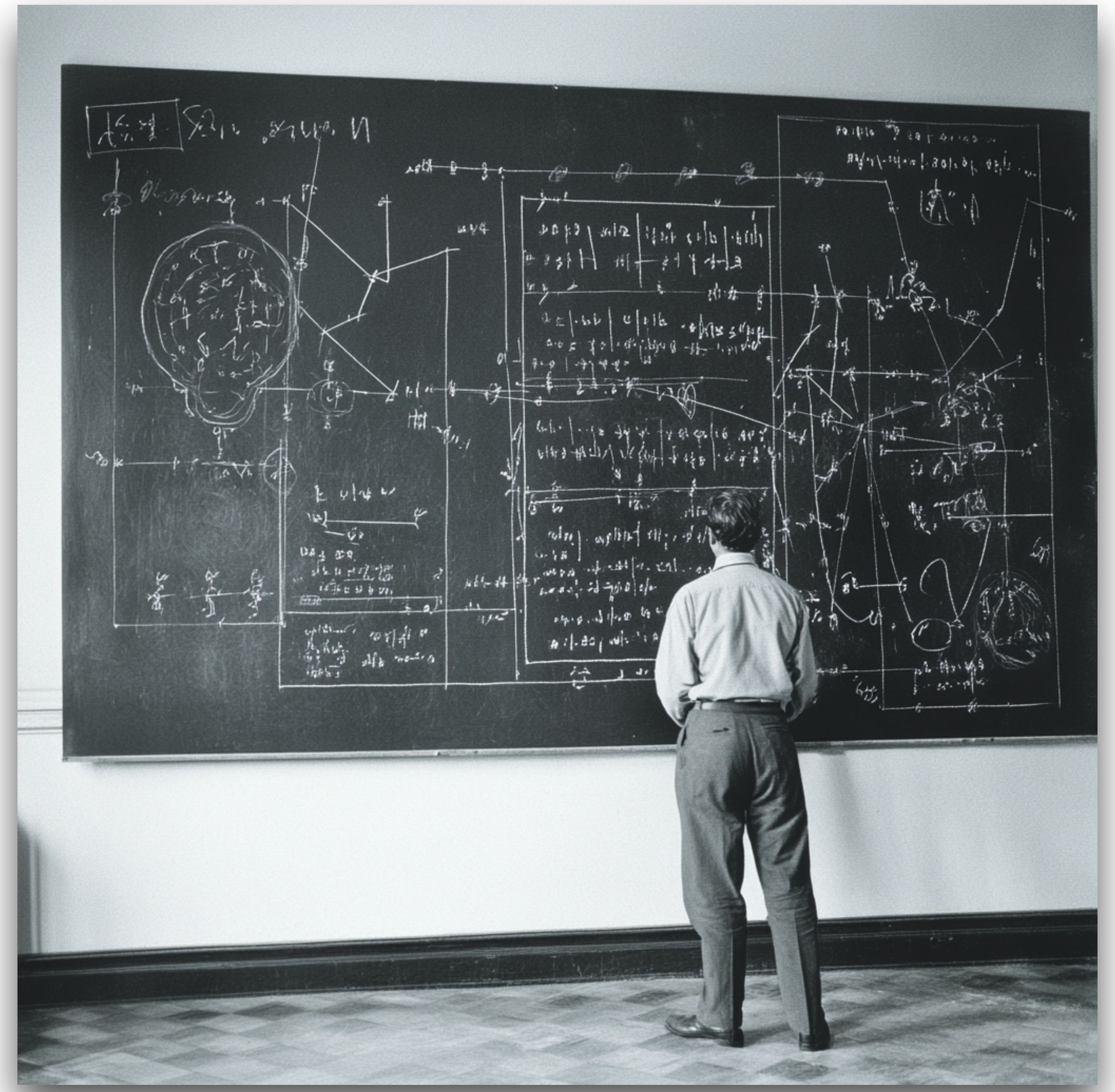
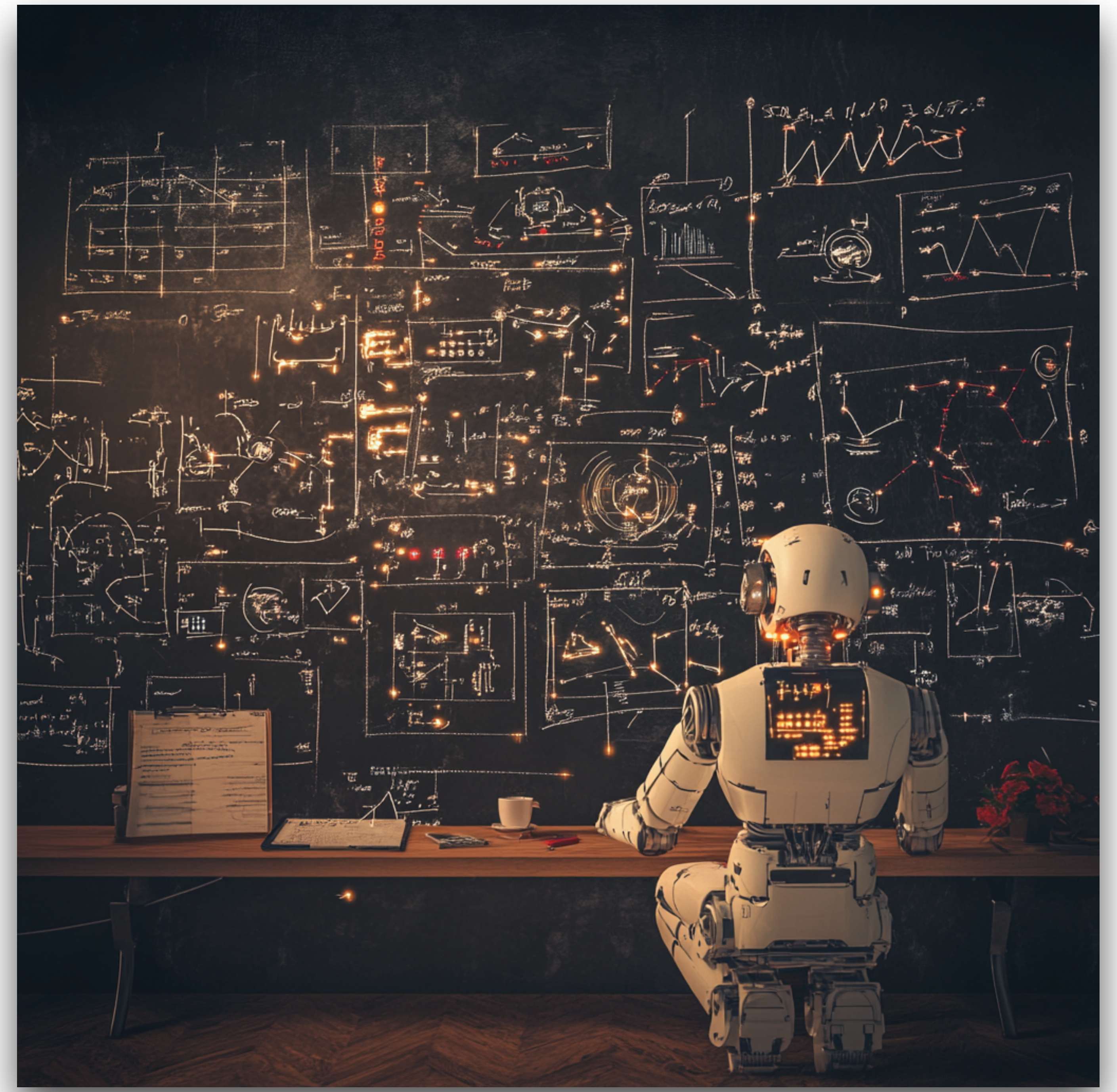
Motivation

- Powerful learners (humans/machines) have **emergent capabilities** that are inherently heuristics—unpredictable by first principle.



Theorists dreaming

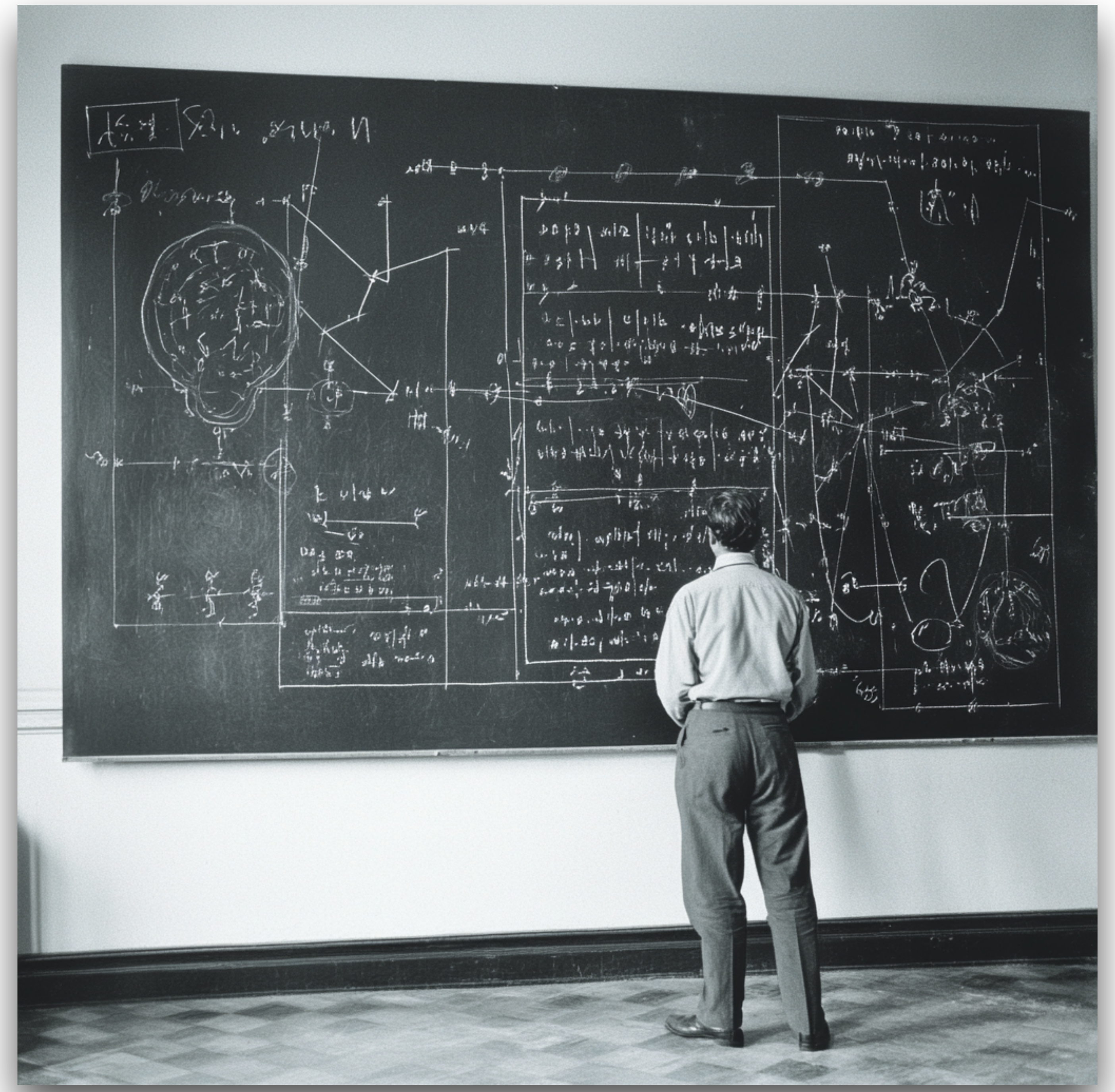
Experimentalists building



AI analyzing

Motivation

- How to design rigorous certification protocols to harness and validate these empirically powerful but heuristic emergent capabilities?



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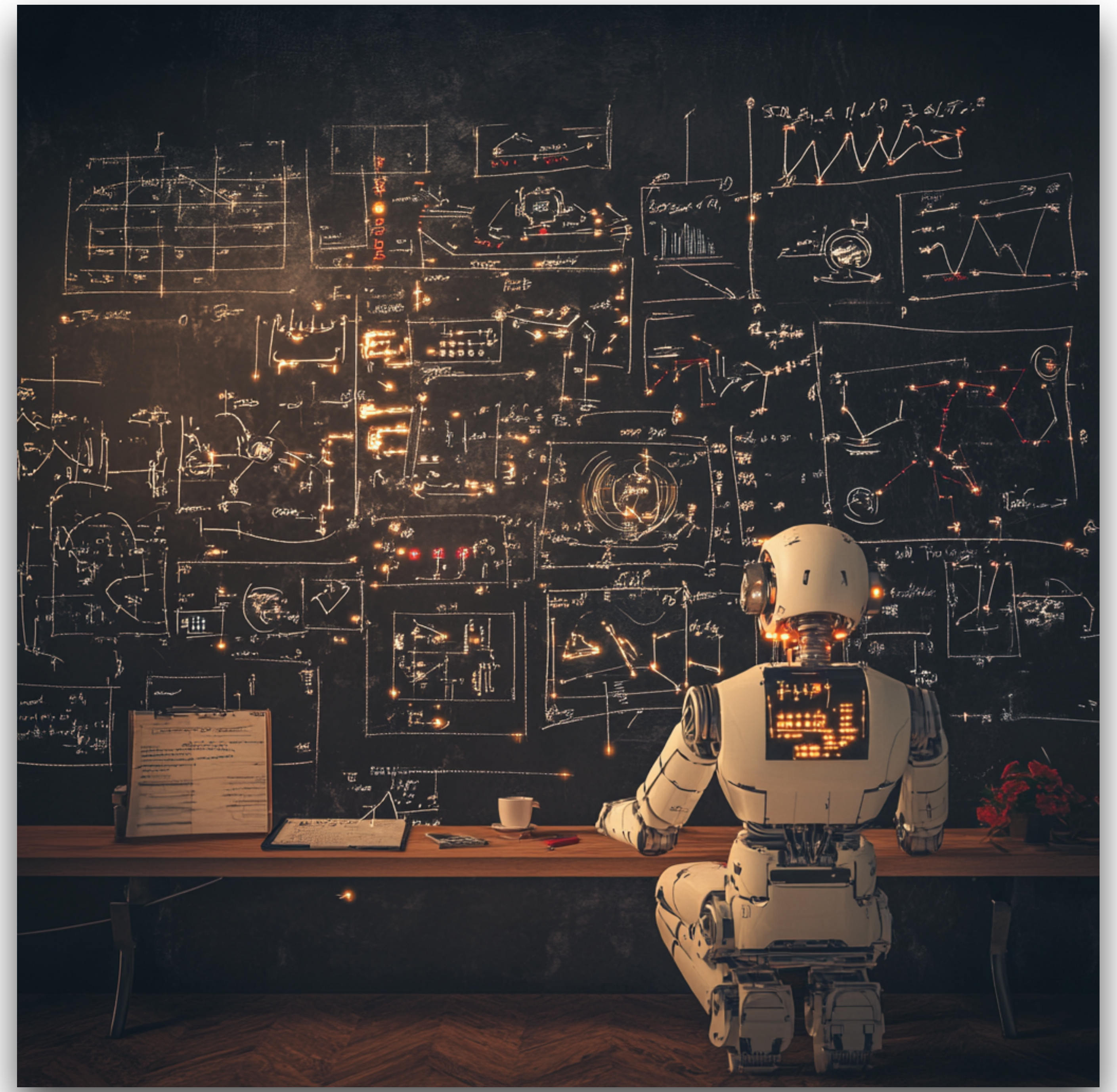
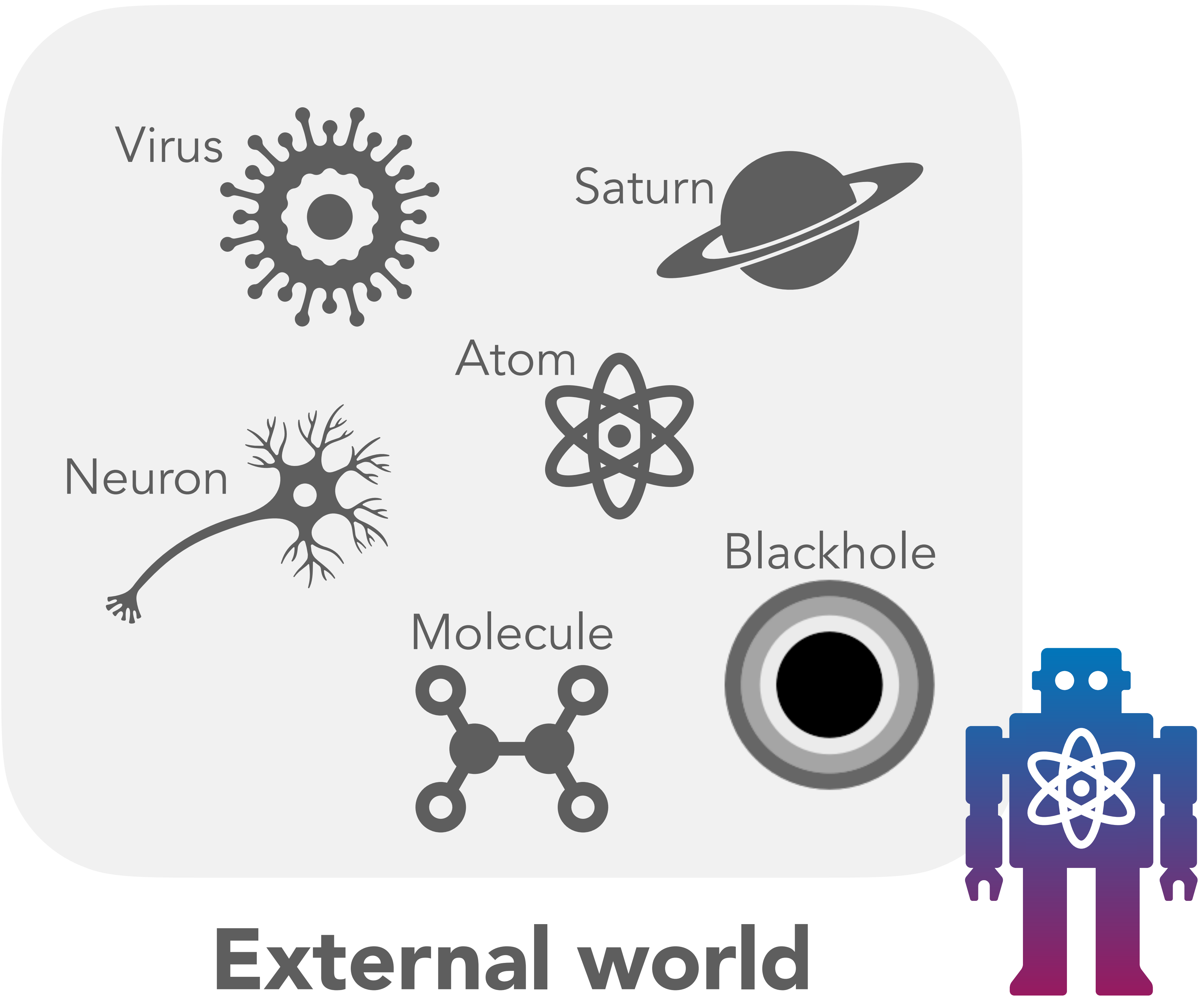


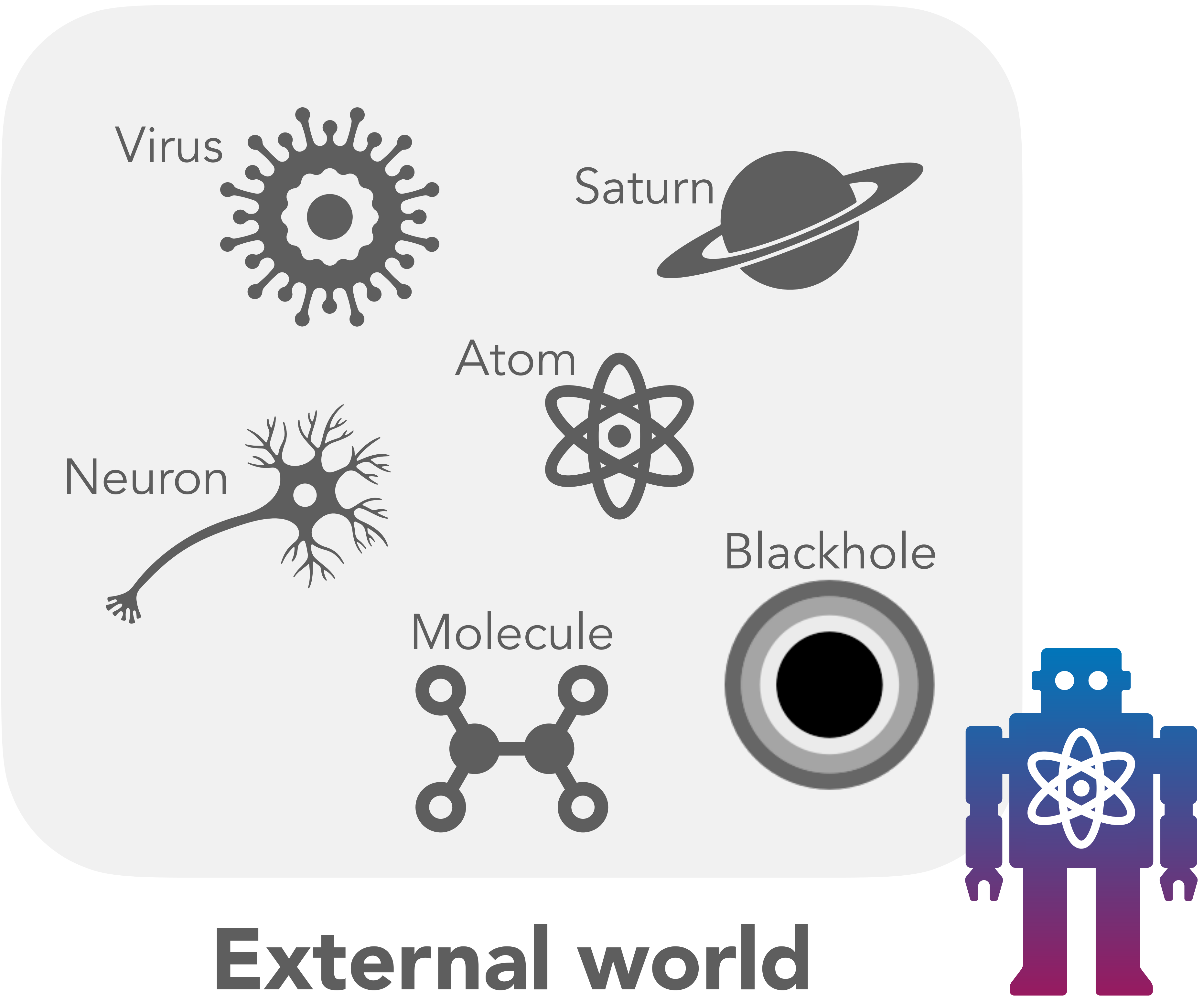
AI analyzing

Two fundamental questions



1. What can/cannot be learned?
2. What can/cannot be certified?

Two fundamental questions



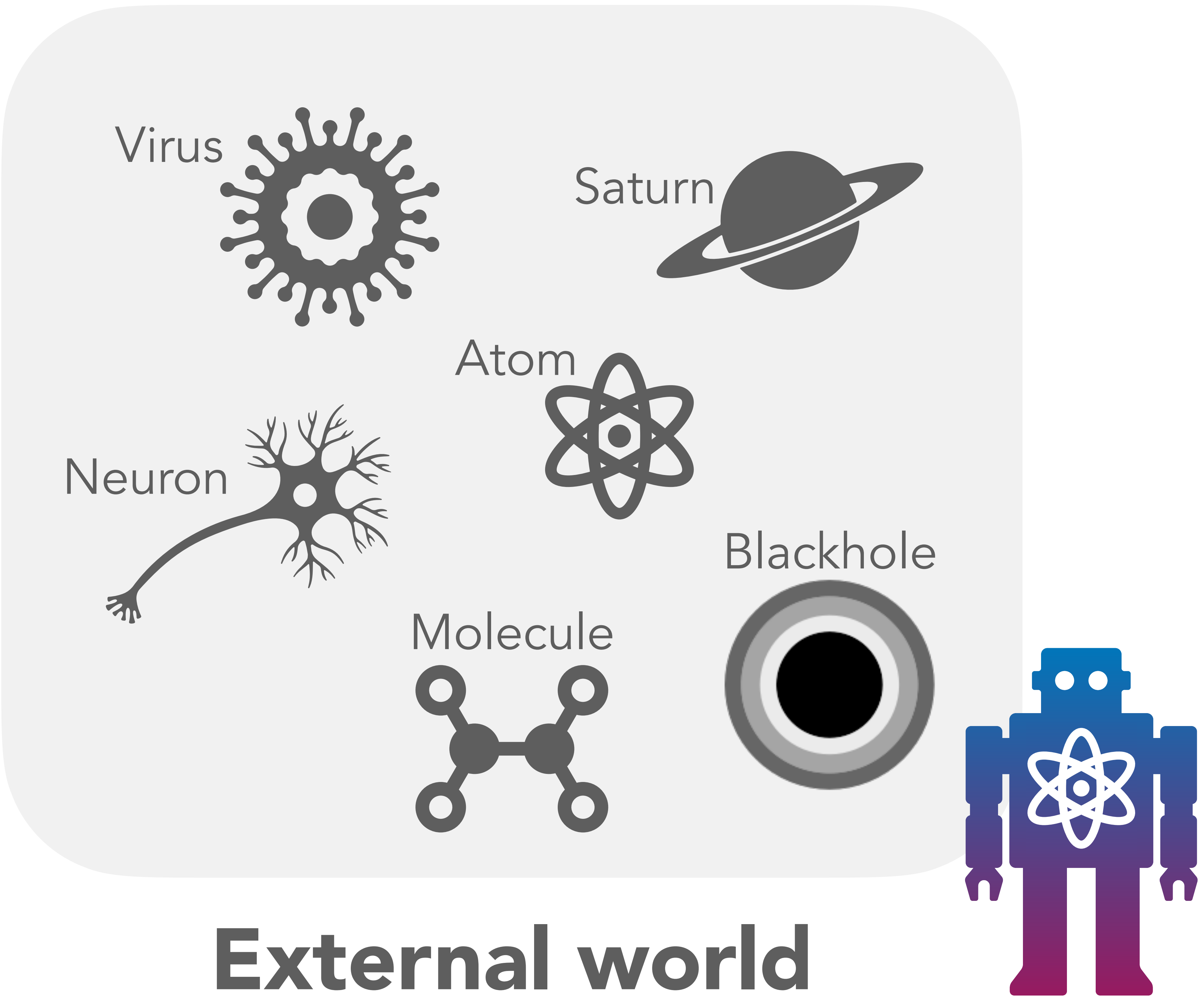
Analog: P

1. What can/cannot be learned?

2. What can/cannot be certified?

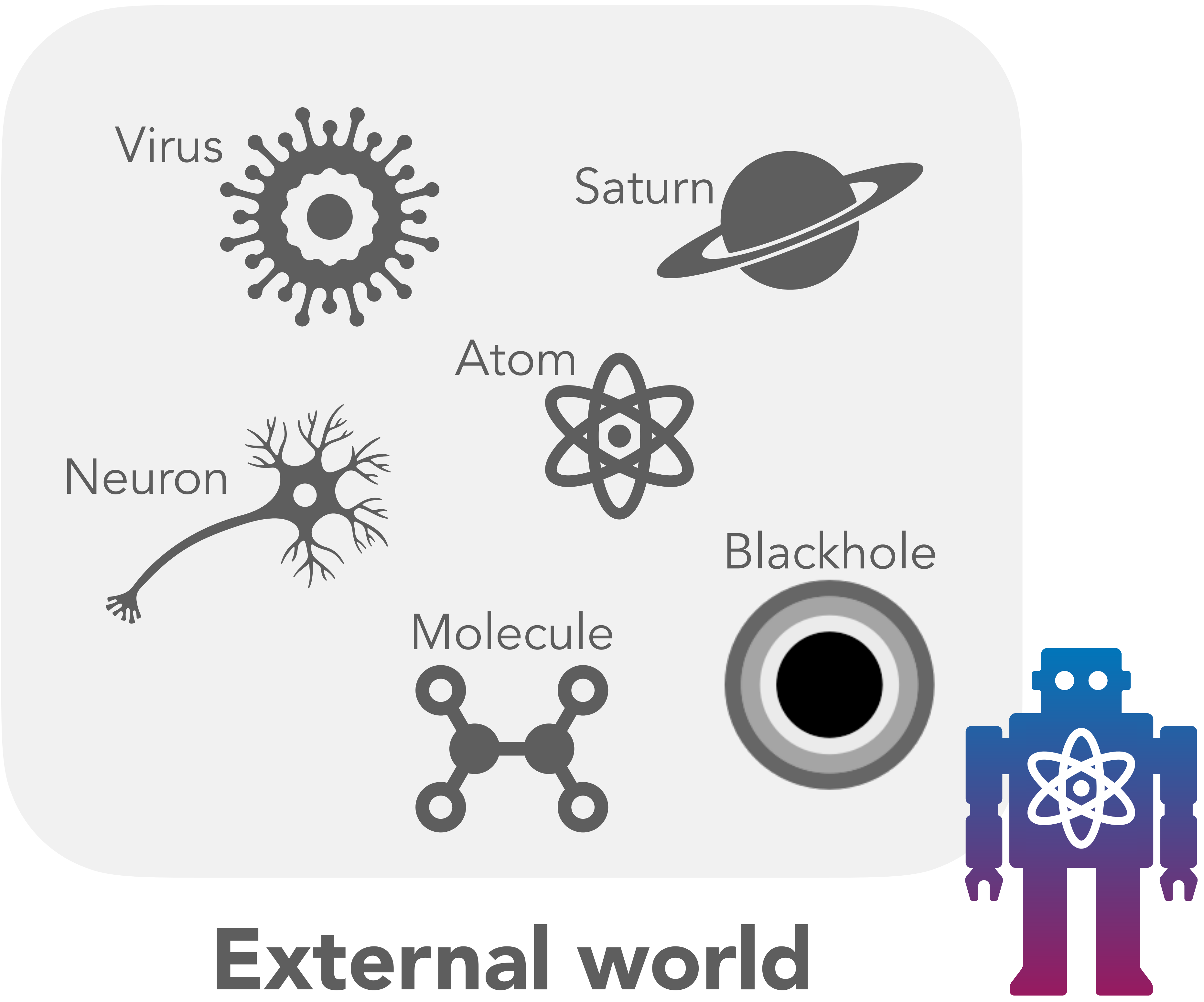
Analog: NP, IP

Two fundamental questions



1. What can/cannot be learned?
2. What can/cannot be certified?

Question: Hamiltonians

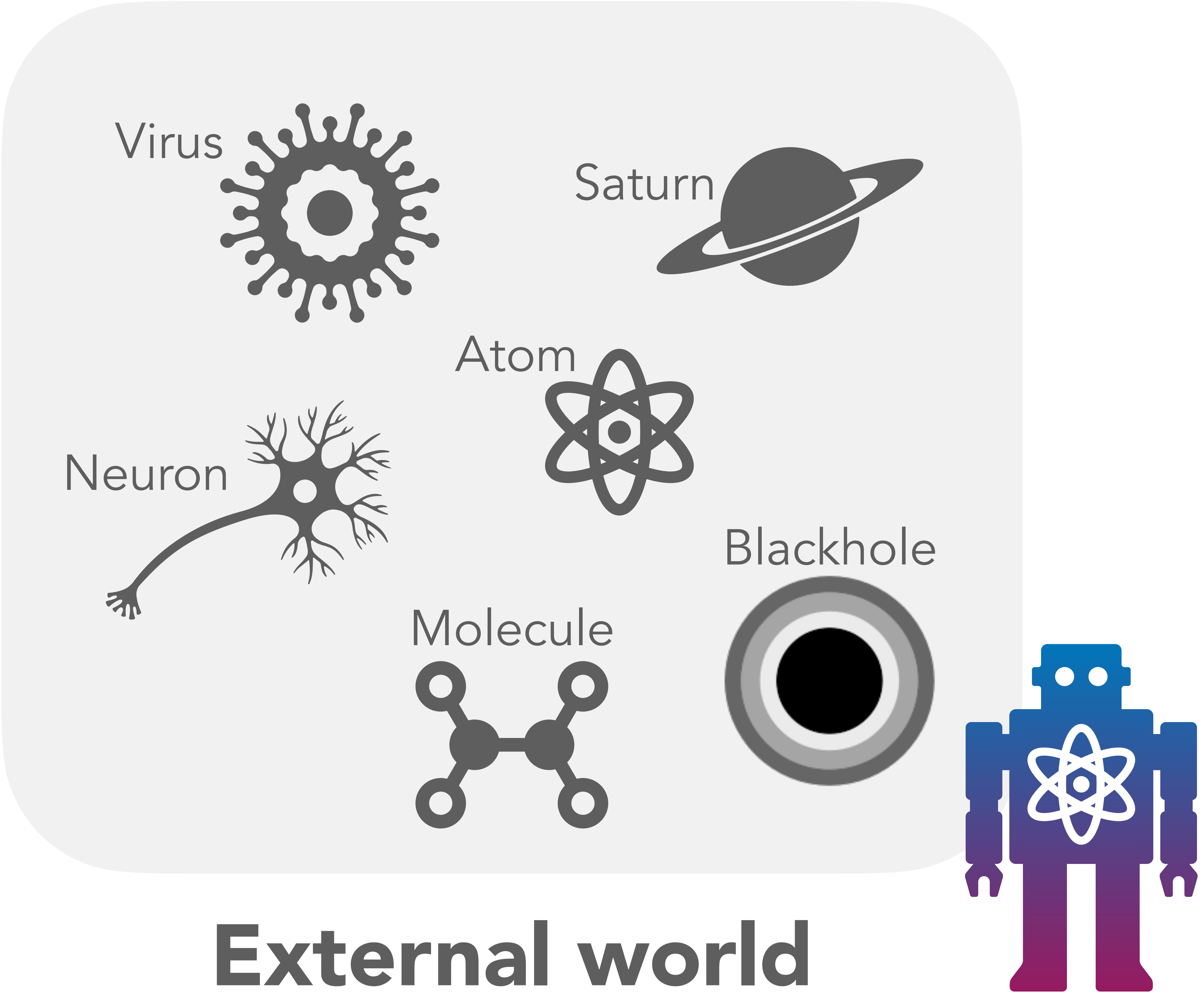


A physical system is described by its **Hamiltonian**.

How to learn Hamiltonian (coefficients, structure, etc.)?

Hint: P44, P46, P77

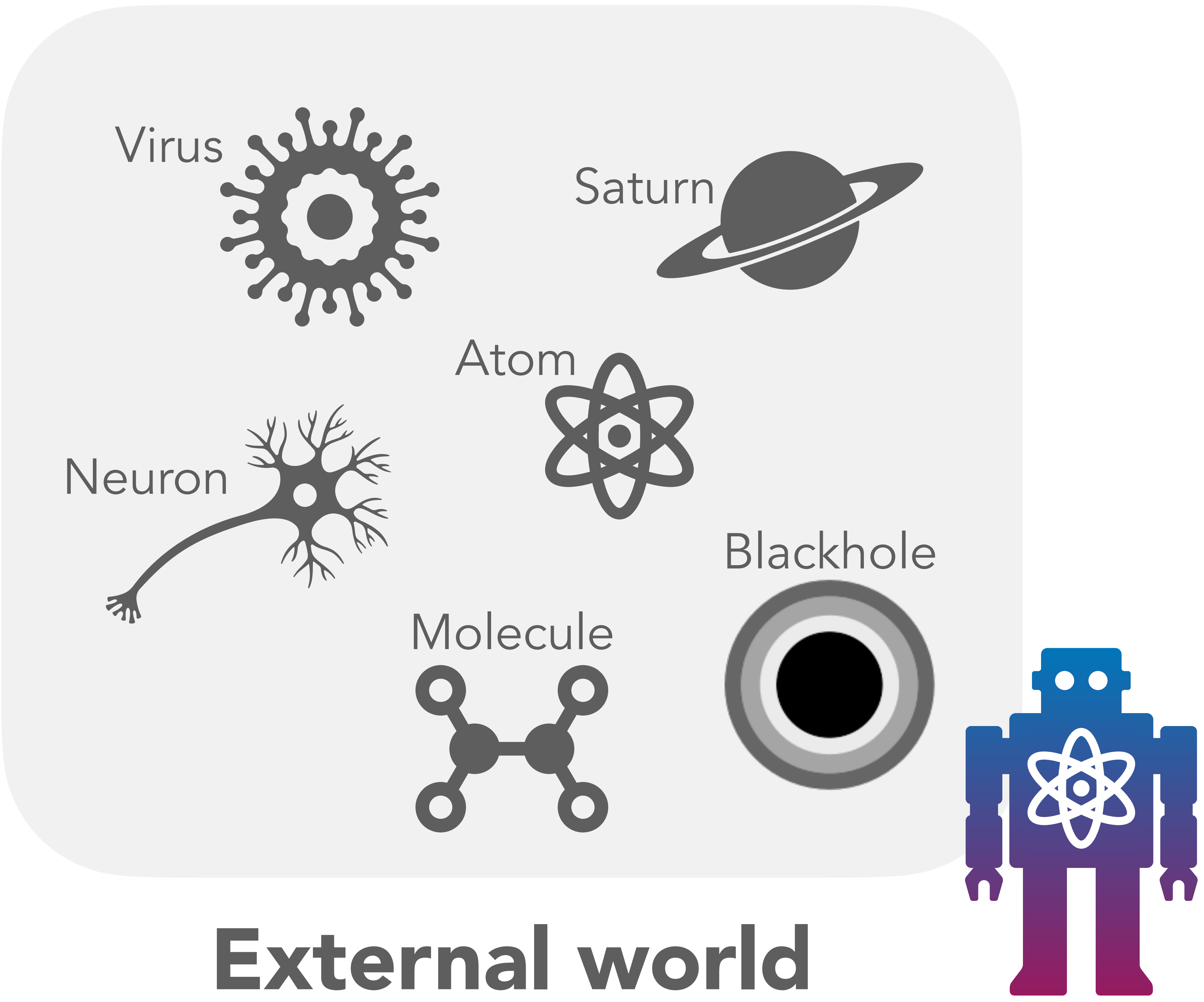
Question: Circuits



How to learn a quantum **circuit** for preparing a state, for evolving under a unitary, etc.?

Hint: P42

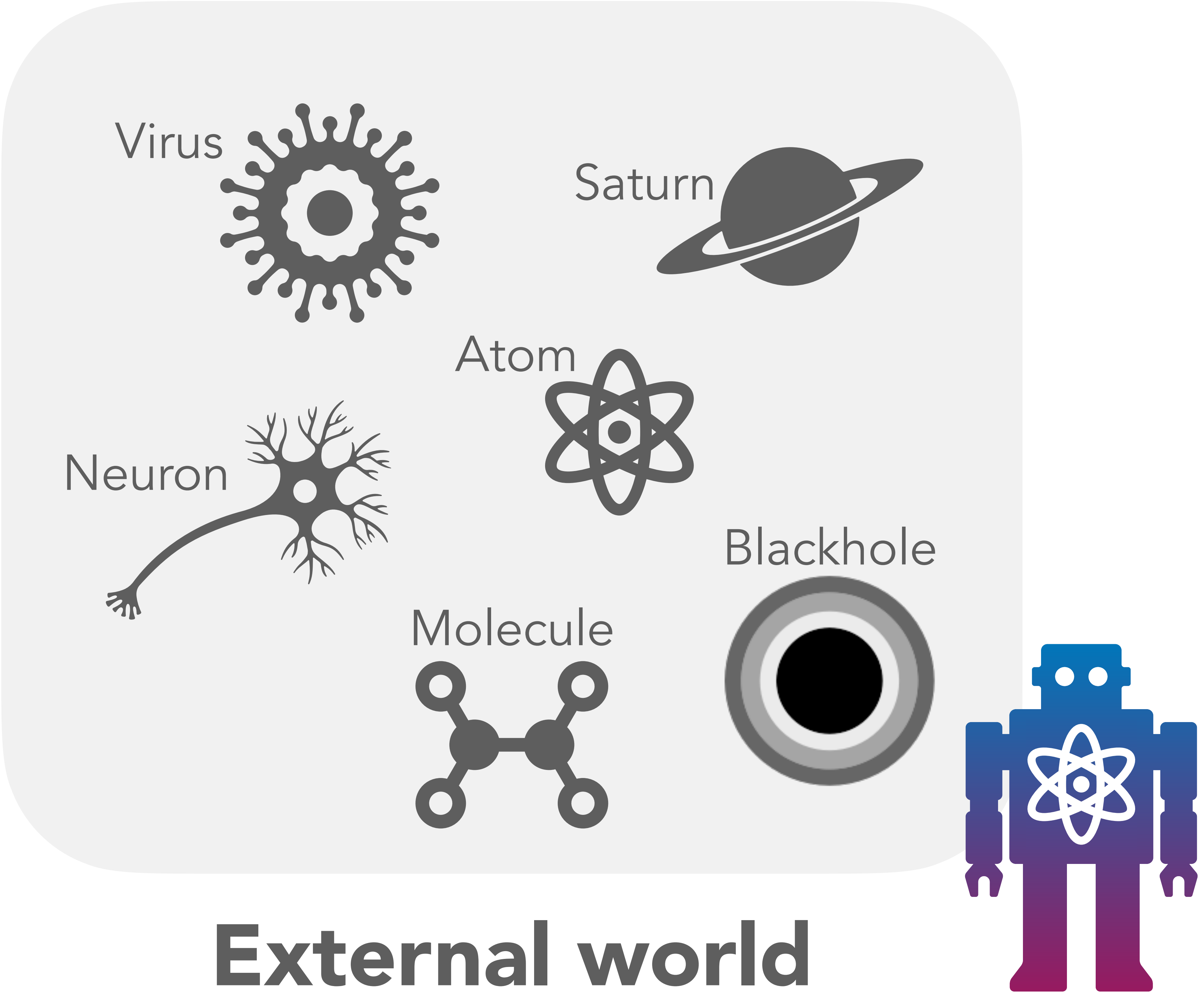
Question: Noise



How to efficiently characterize the **noise** in a quantum device?

Hint: P92

Question: Boson/Fermion

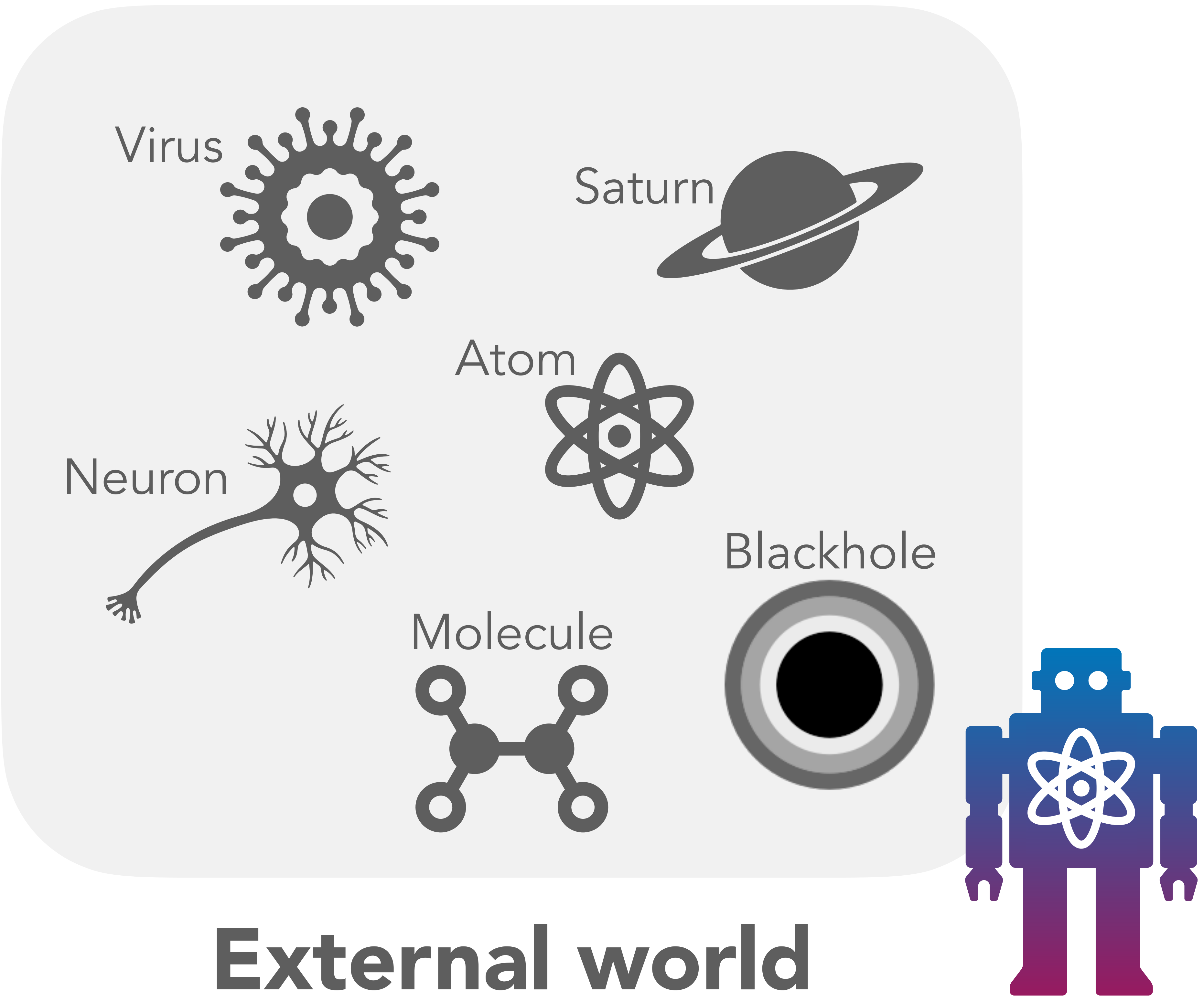


Most physical systems are **not** consisted of qubits.

How to efficiently learn systems of **bosons/fermions**?

Hint: P87, P114

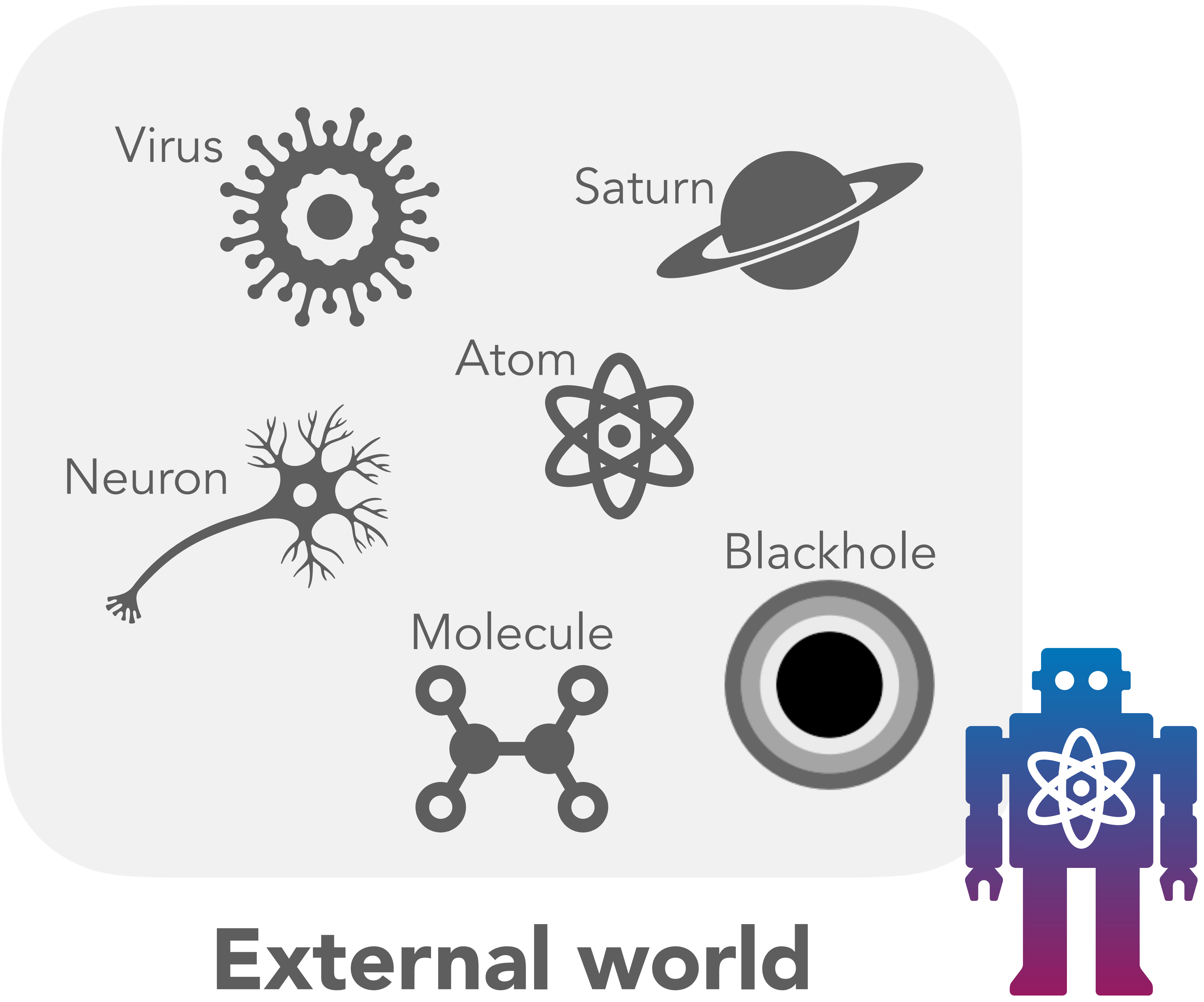
Question: Approximate Model



How to learn the closest **approximate model** describing the underlying physics?

Hint: S2

Question: Hardness

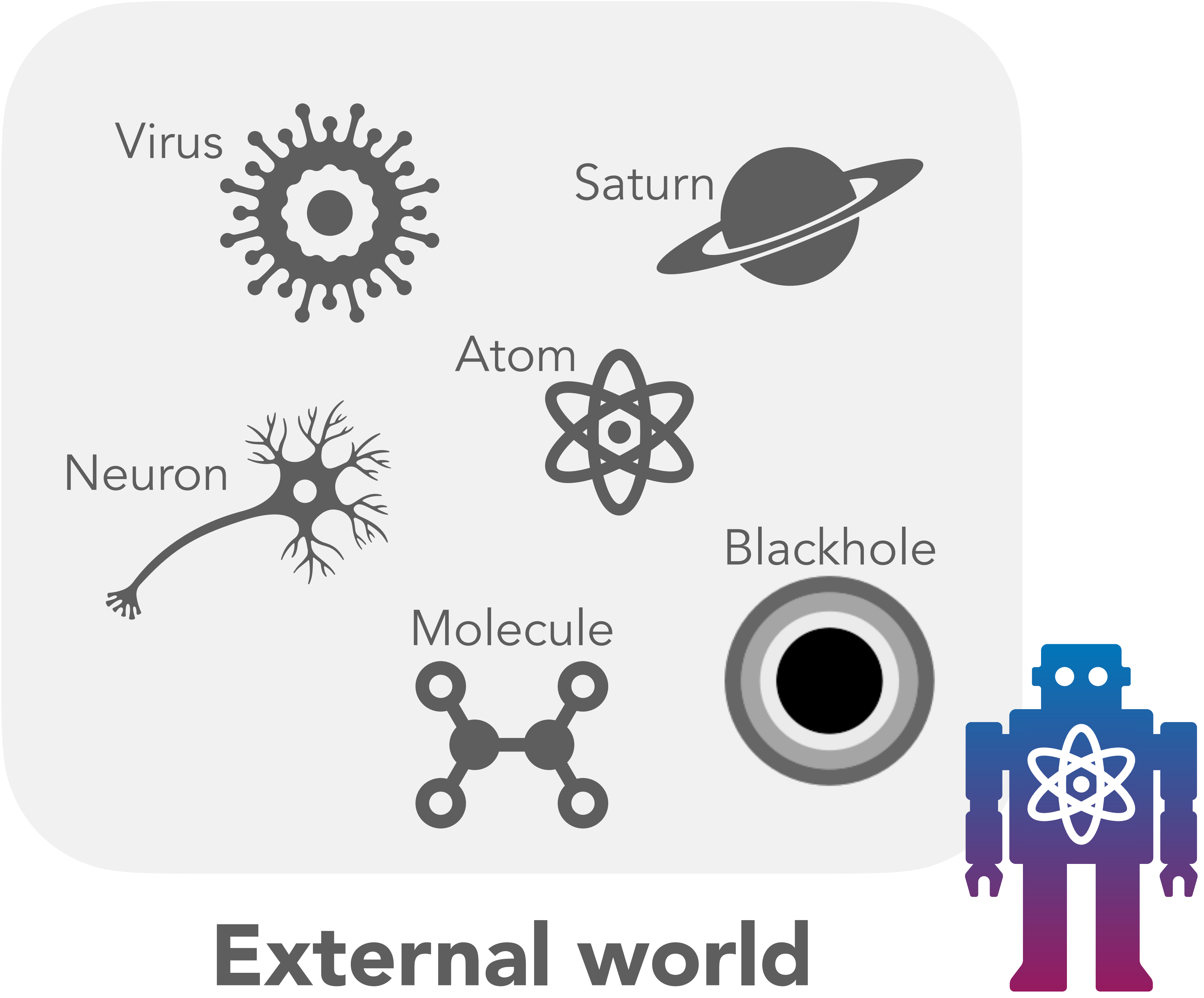


Are basic physical properties fundamentally **hard to learn**?

(time, causal cone, topological order, entanglement)

Hint: L6, S6, P104

Two fundamental questions



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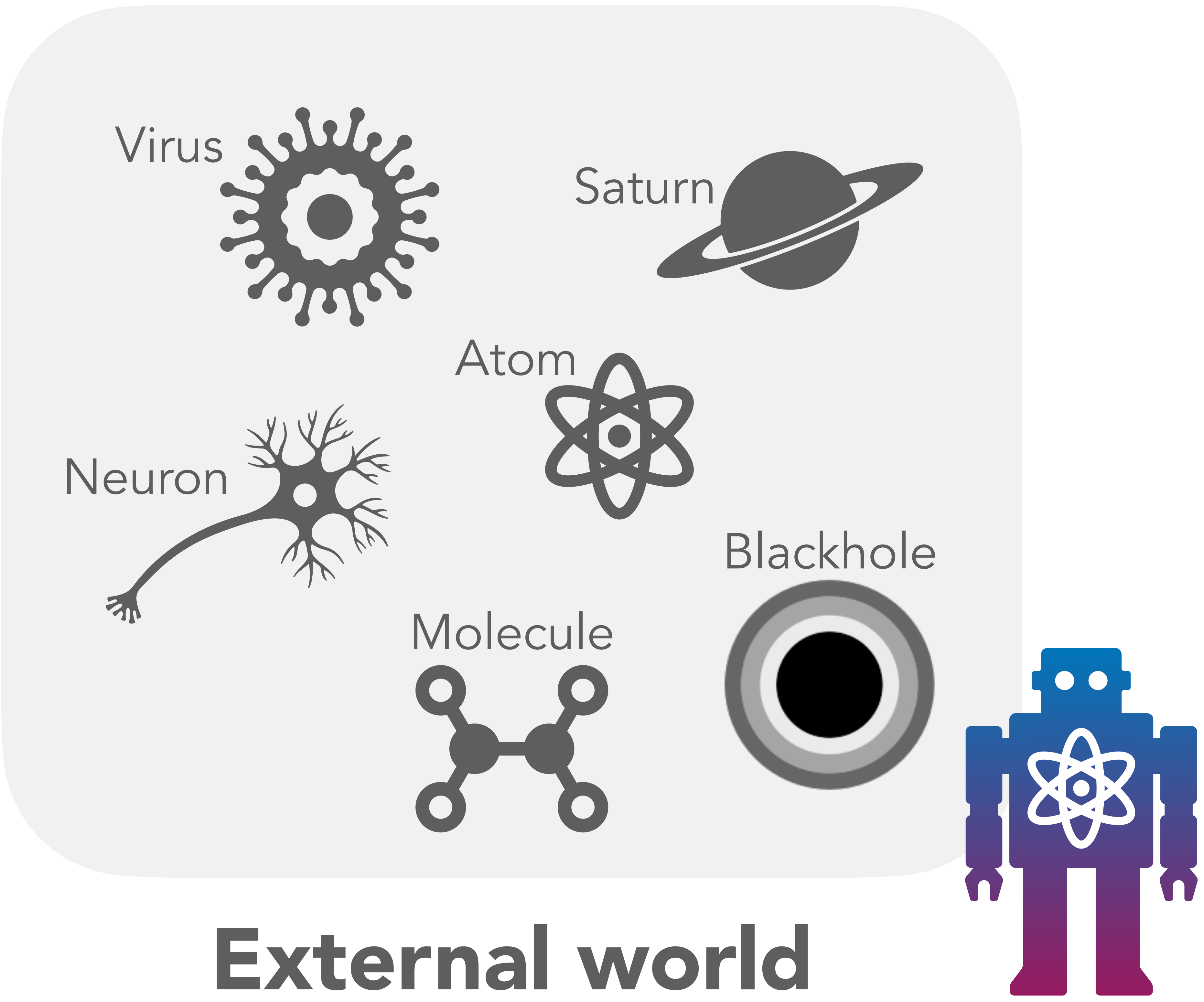
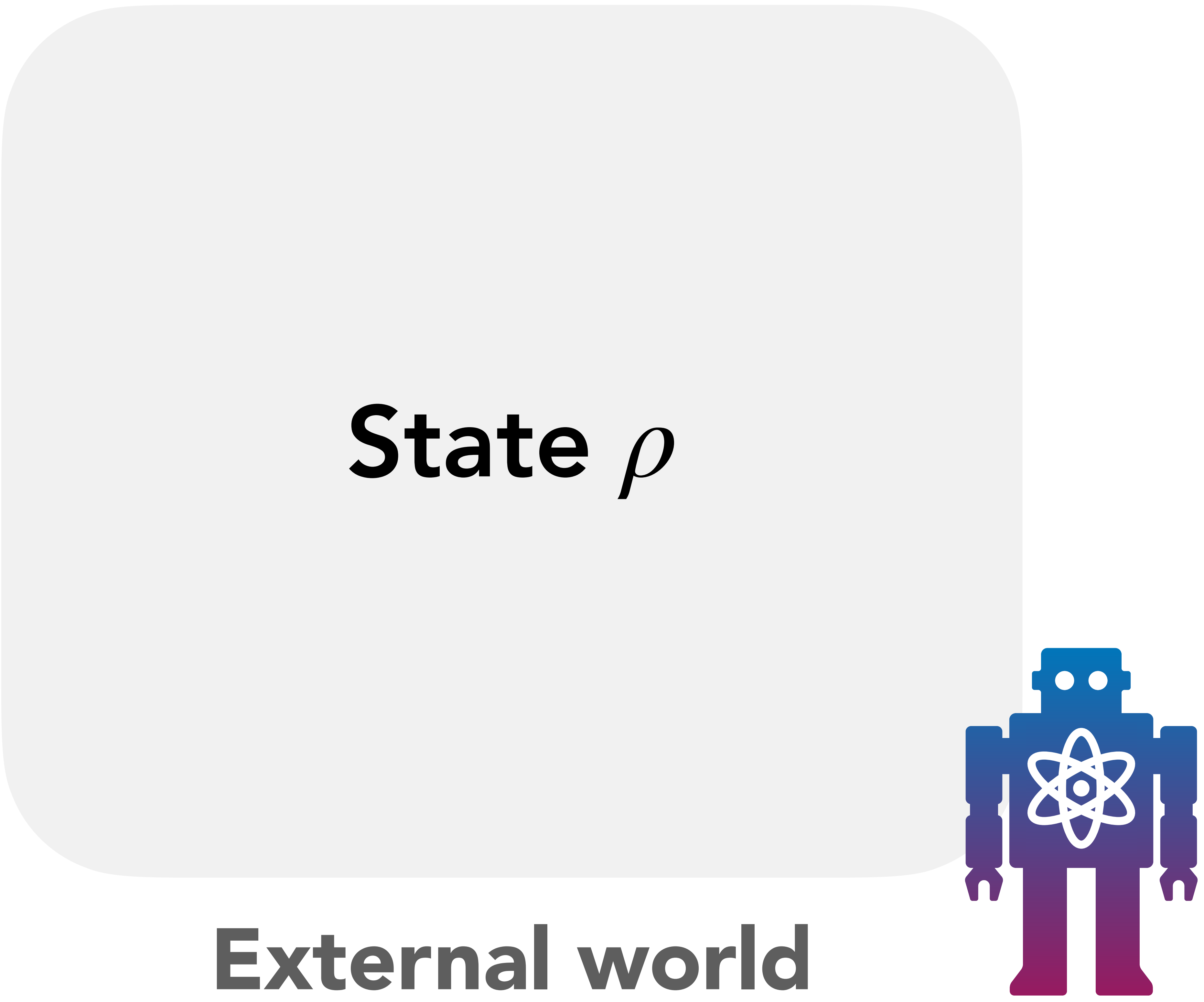
Two fundamental questions



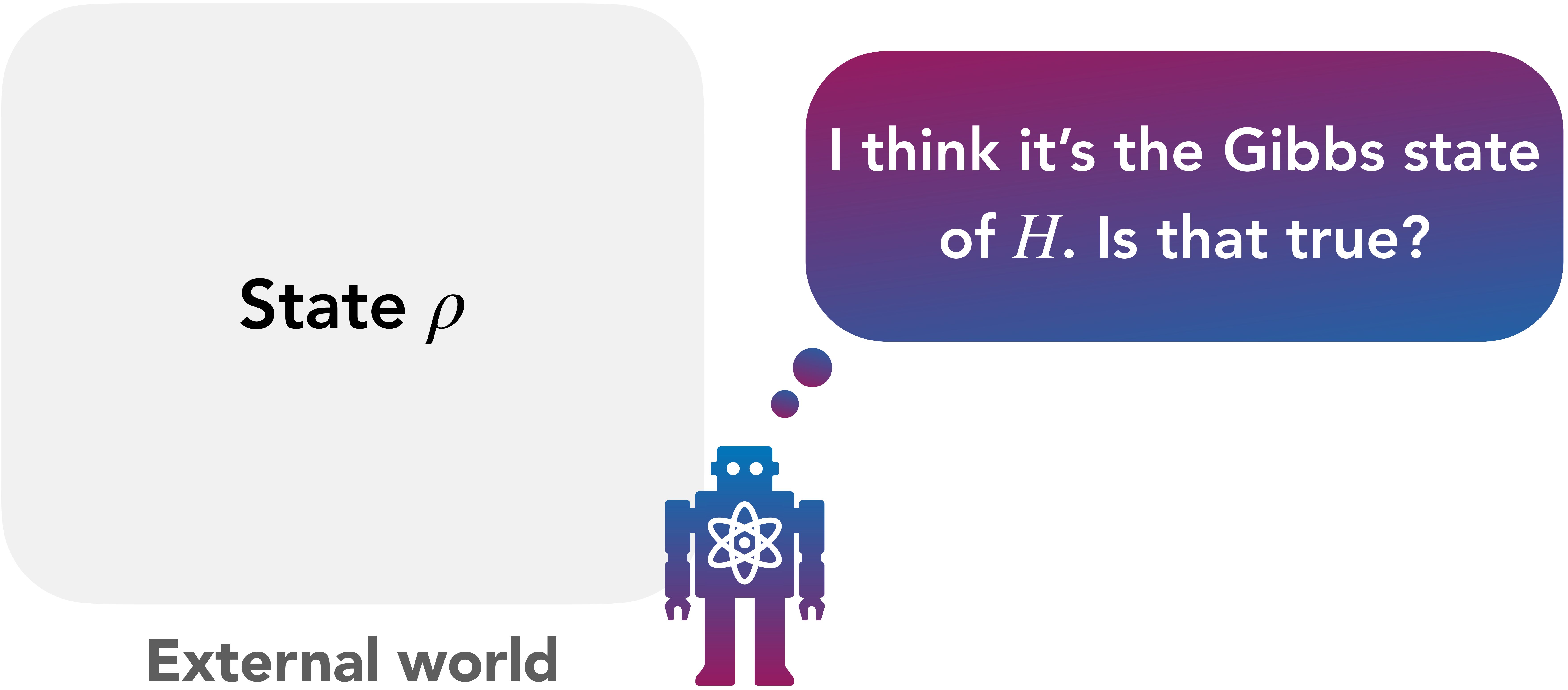
1. What can/cannot be learned?
2. What can/cannot be certified?

A useful playground



1. What can/cannot be learned?
2. What can/cannot be certified?

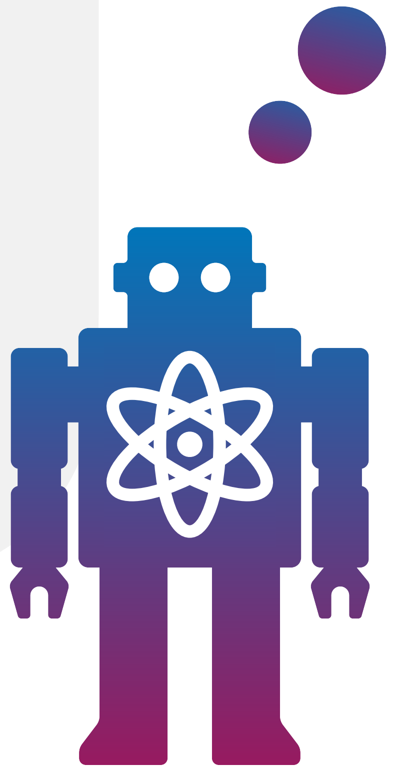
Certifying Gibbs Sampling



Certifying State Prep

State ρ

External world



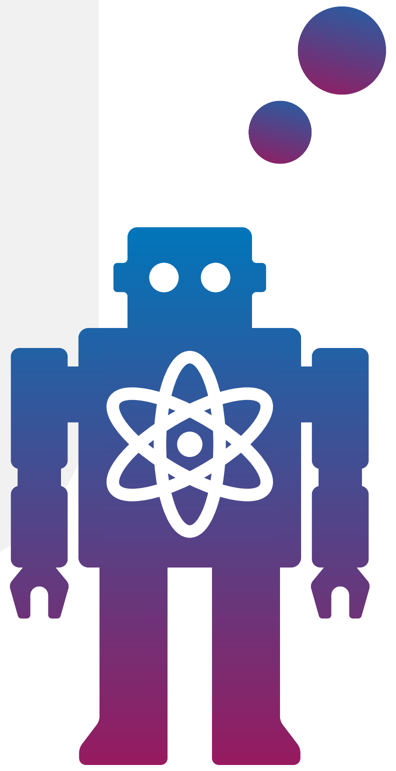
I think it's the Gibbs state of H. Is that true?

I try to create $|\psi\rangle$ in the lab. Did I succeed?

Certifying Heuristic AI

State ρ

External world



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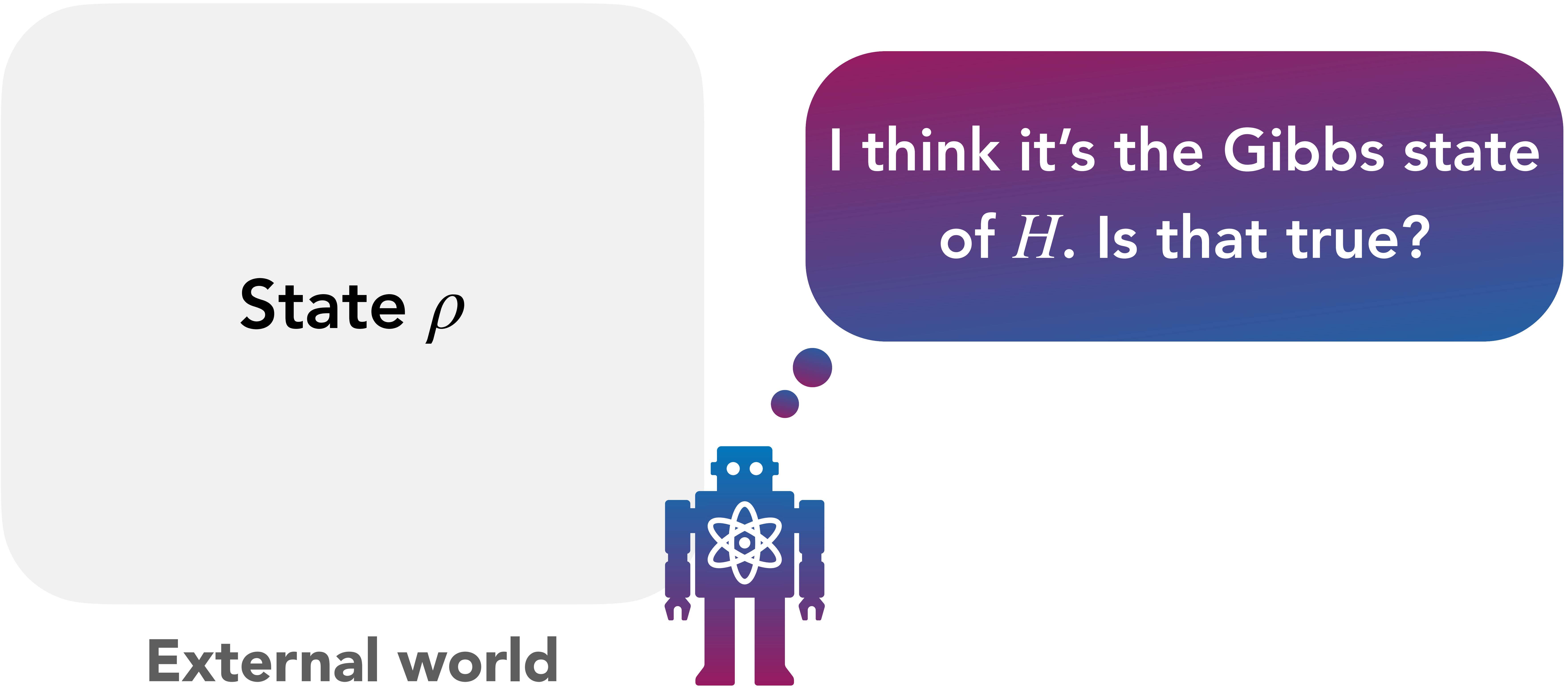
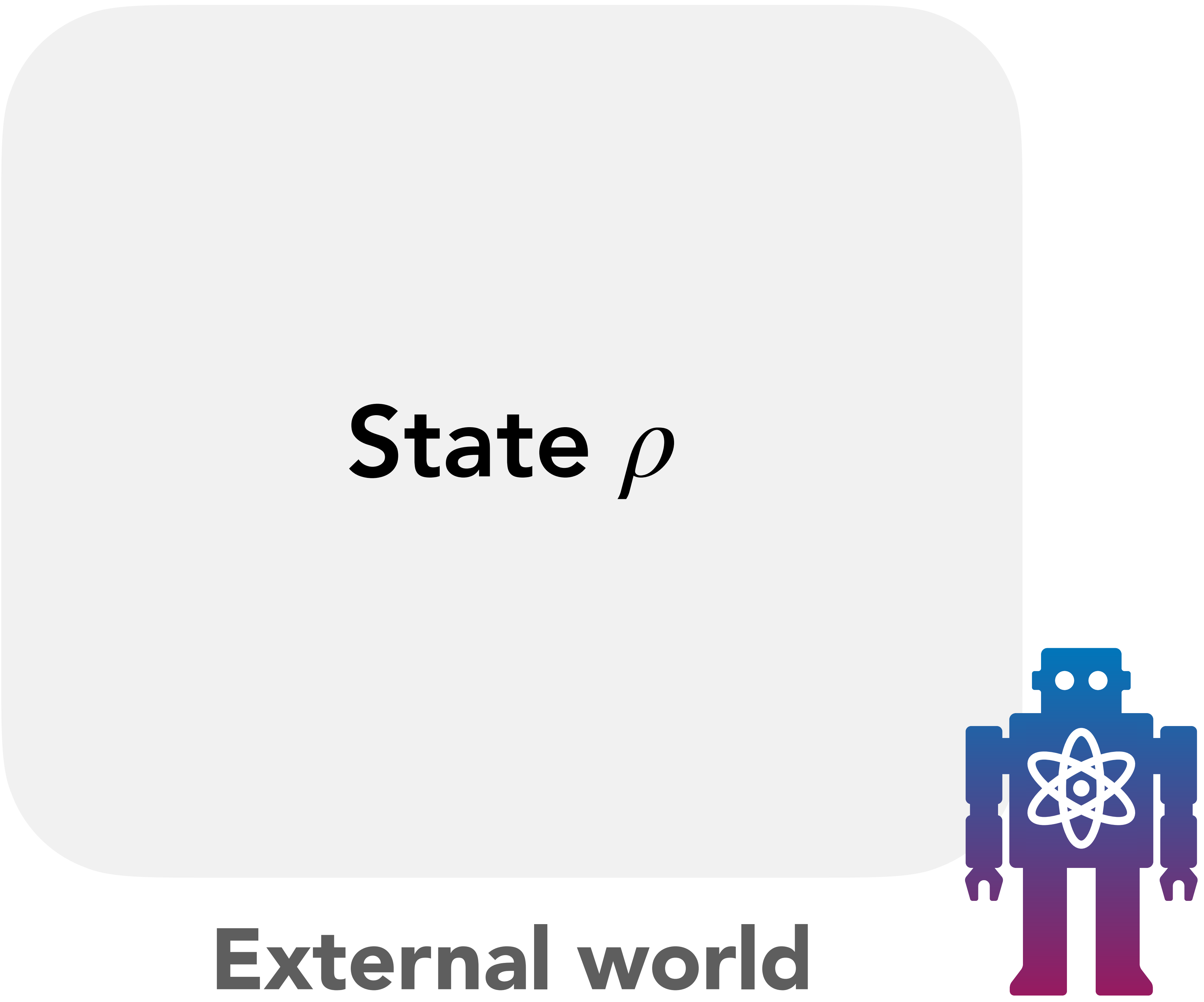


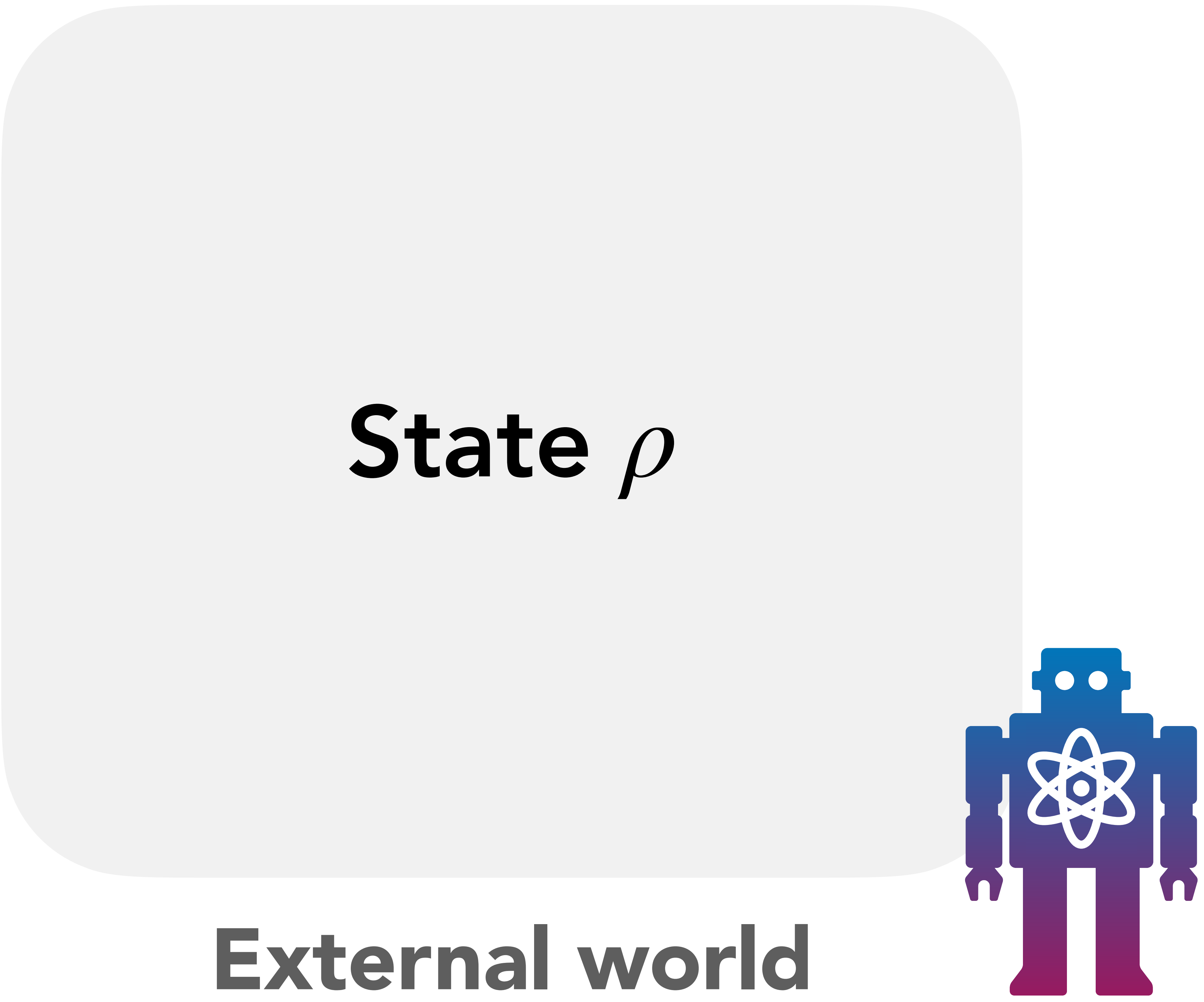
Question: High temperature



Given a local H.

Can the AI agent efficiently certify that ρ is close to a **high-temperature Gibbs state** of H?

Question: High temperature



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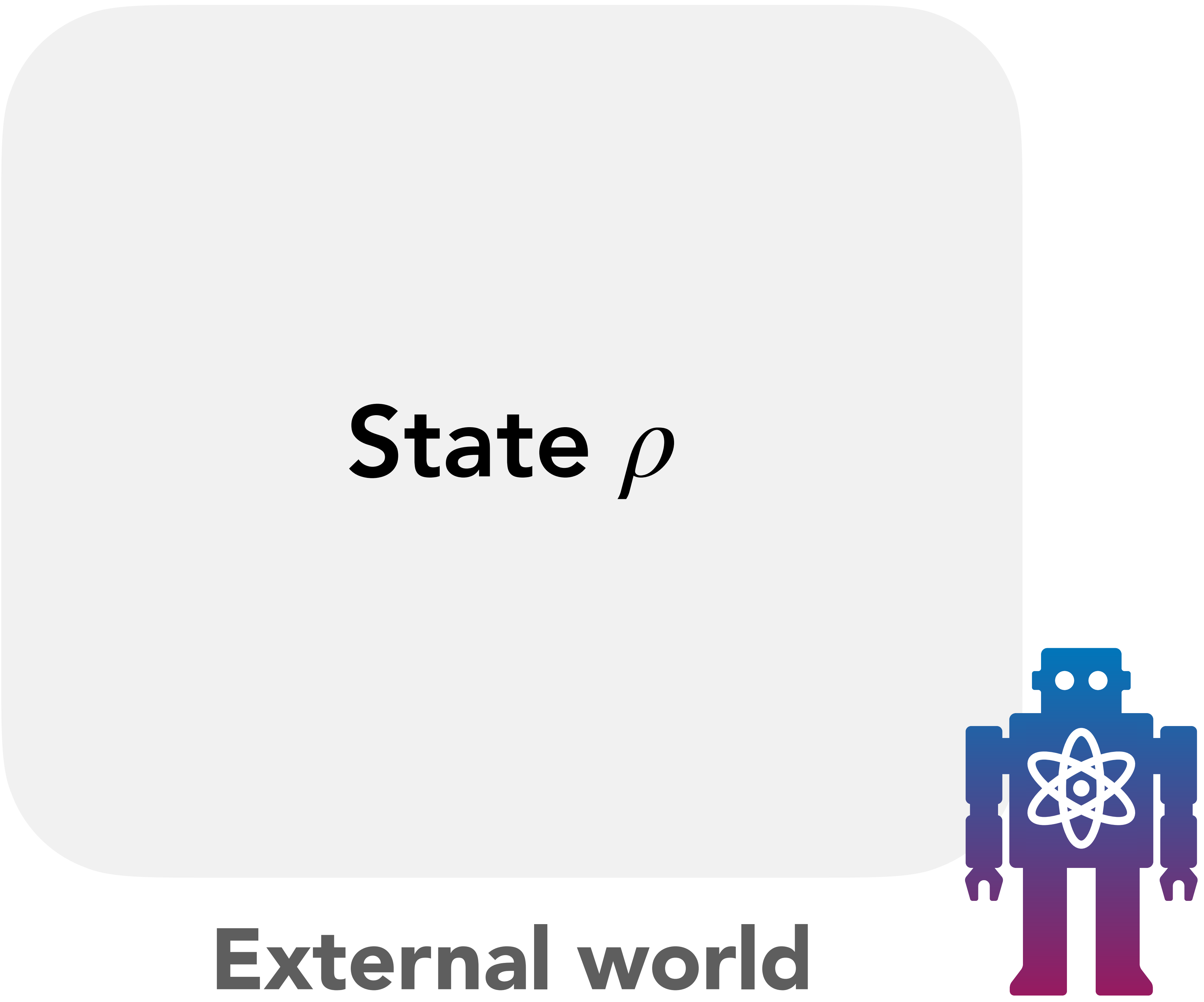

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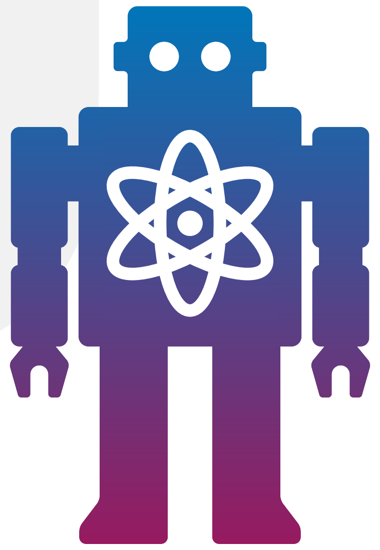
Can the AI agent efficiently certify that ρ is close to a **high-temperature Gibbs state** of H?

Hint 1: No.

Question: High temperature

State ρ

External world



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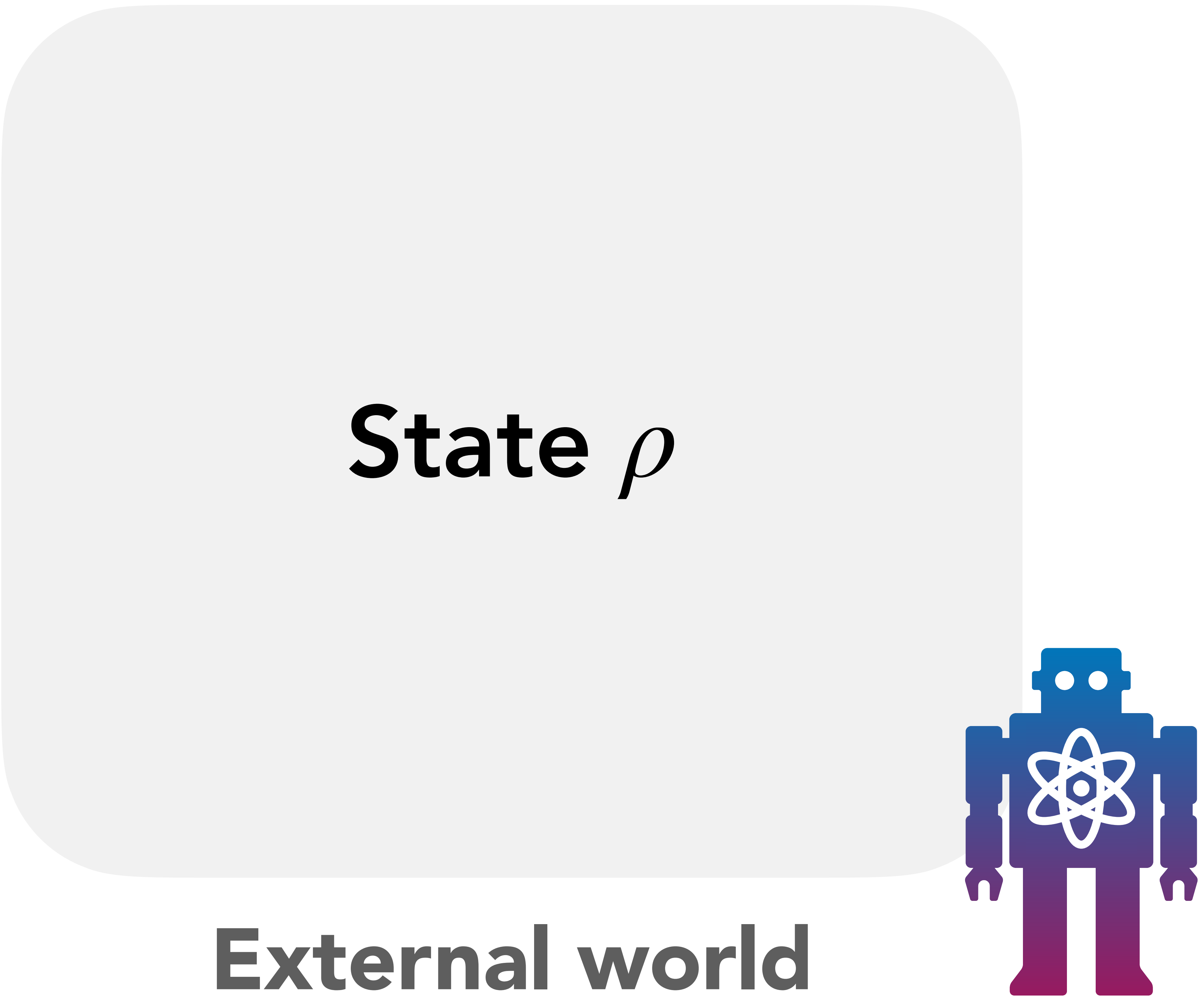
Can the AI agent efficiently certify that ρ is close to a **high-temperature Gibbs state** of H?

Hint 1: No.

Hint 2: Think about ∞-temperature states.

Question: High temperature



Given a local H.

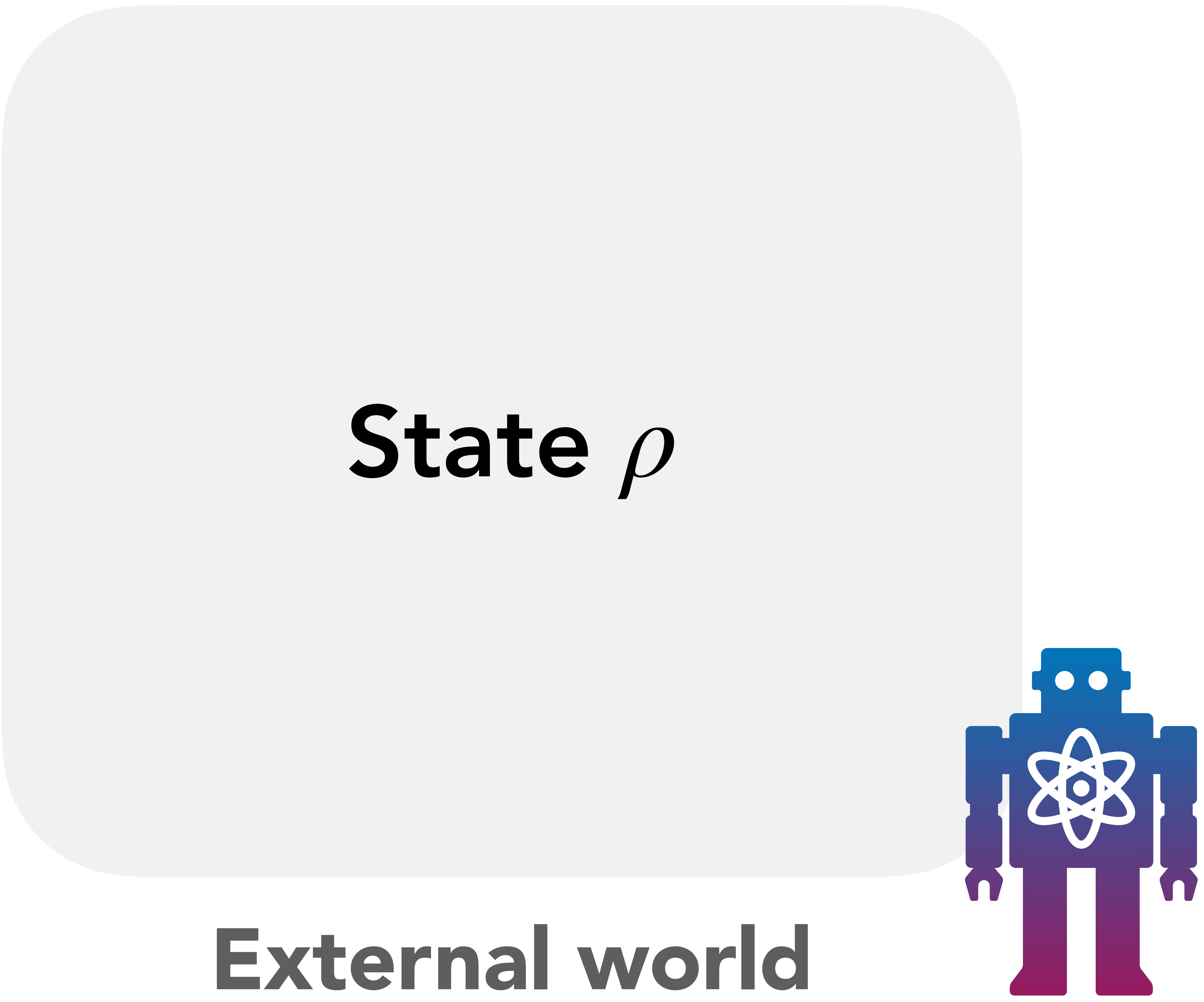
Can the AI agent efficiently certify that ρ is close to a **high-temperature Gibbs state** of H?

Hint 1: No.

Hint 2: Think about ∞-temperature states.

Hint 3: Hardness of estimating entropy.

Question: Low temperature



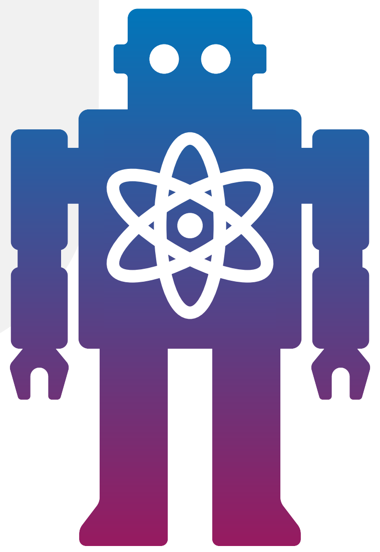
Given a local H.

Can the AI agent efficiently certify that ρ is close to the **ground state** of H (in energy)?

Question: Low temperature

State ρ

External world



Given a local H.

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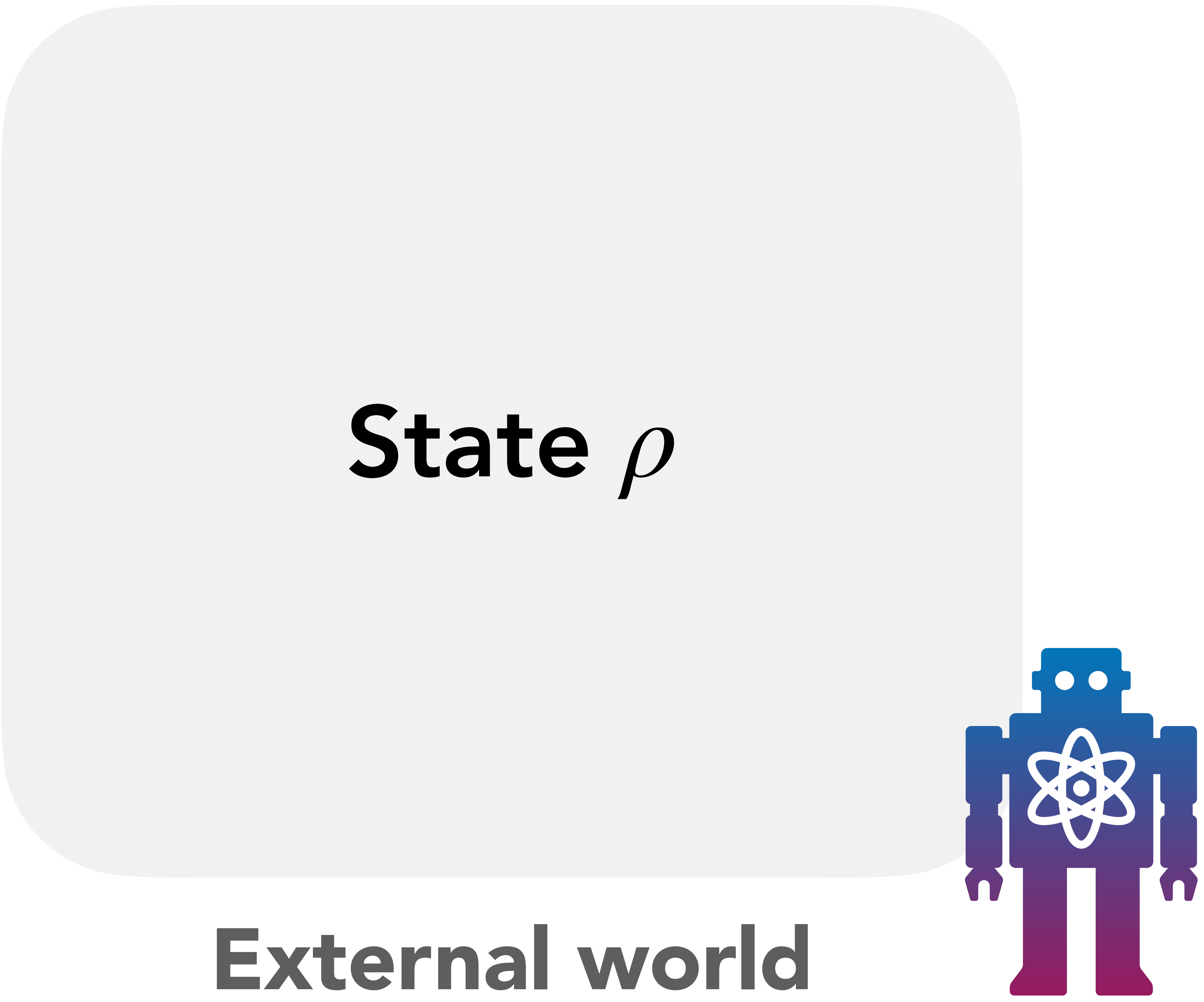
Hint 1: No.

Question: Low temperature



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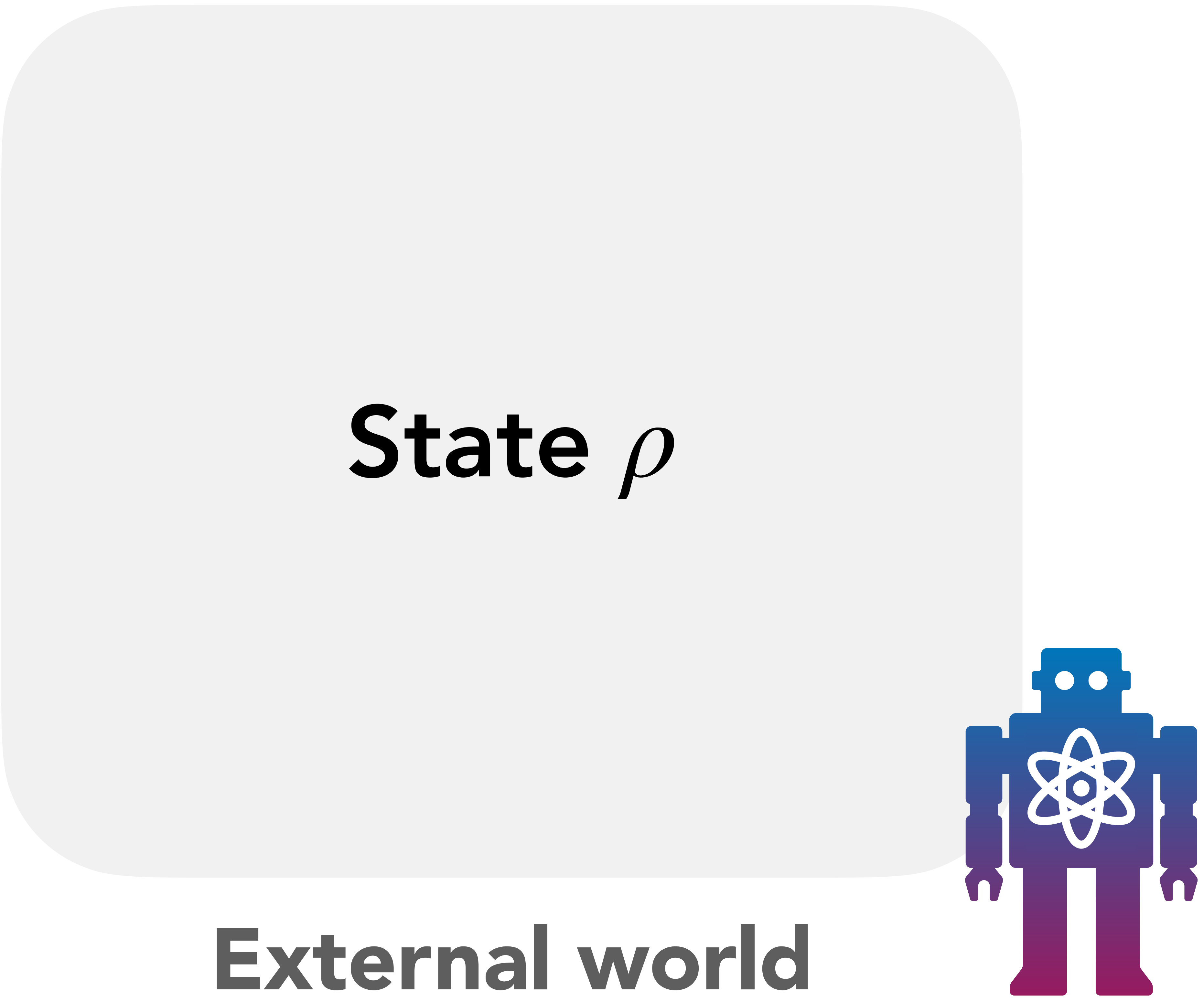
Can the AI agent efficiently certify that ρ is close to the **ground state** of H (in energy)?

Hint 1: No.
Hint 2: Take any hard H.

Question: Low temperature



Given a local H.

Can the AI agent efficiently certify that ρ is close to the **ground state** of H (in energy)?

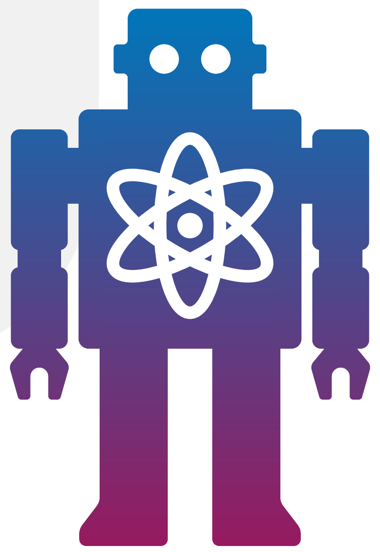
Hint 1: No.
Hint 2: Take any hard H.
Hint 3: Put a local min w. fine-tuned energy.

Certifying Gibbs Sampling

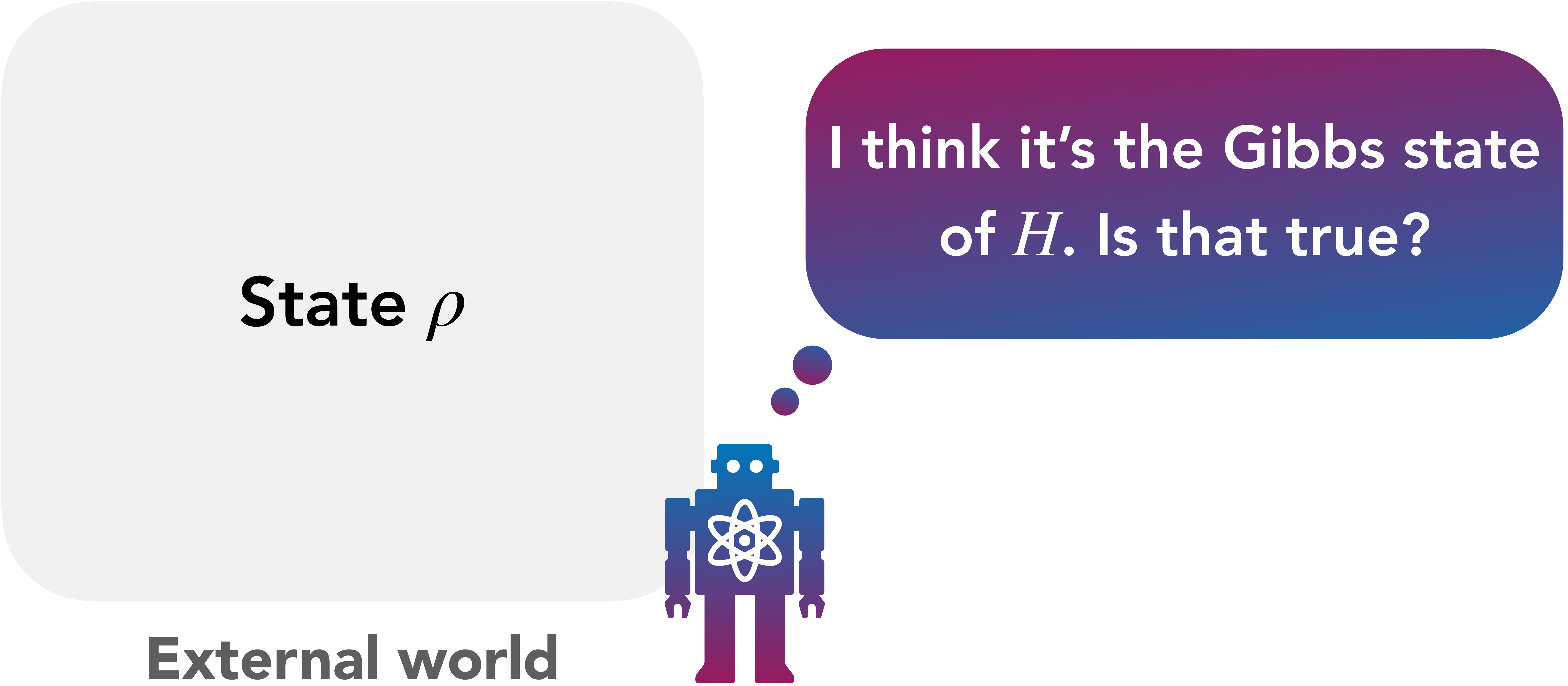
State ρ

External world

I think it's the Gibbs state of H. Is that true?



Certifying Gibbs Sampling

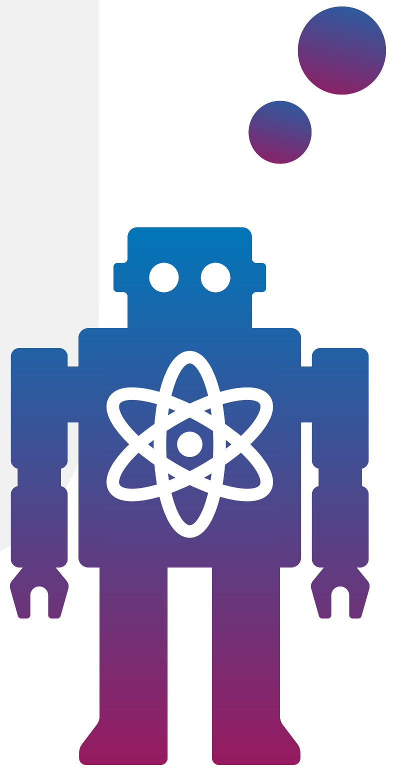


Hard for both low and high temperatures

Certifying State Prep

State ρ

External world



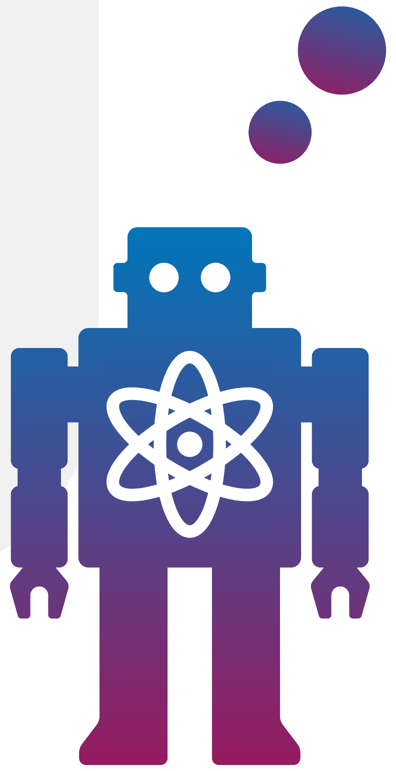
I try to create $|\psi\rangle$ in the lab. Did I succeed?

What about this?

Certifying Heuristic AI

State ρ

External world



Or this?

My trained AI says the state is $|\psi\rangle$. Is that right?

State Certification

- We have a desired n-qubit state $|\psi\rangle$, which is our target state.
- We have an n-qubit state ρ created in the experimental lab.
- **Task:** Test if ρ is close to $|\psi\rangle\langle\psi|$ or not.

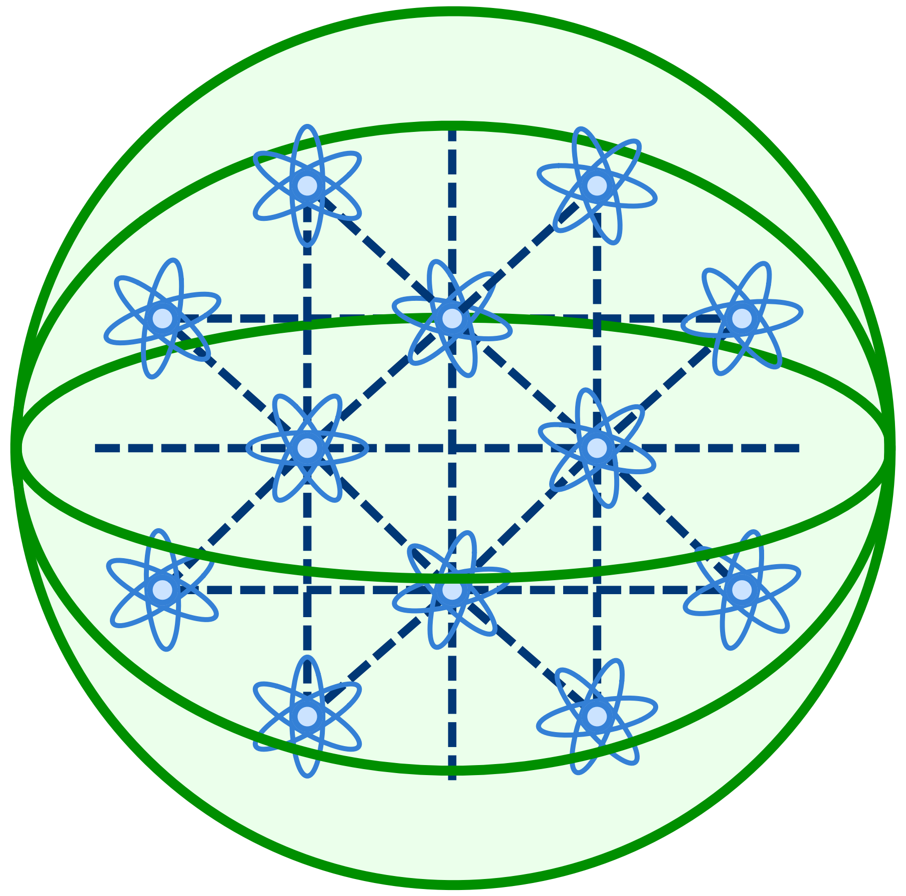
  ($\langle\psi|\rho|\psi\rangle$ is close to 1)

How to Certify?

- **Approach 0:** Direct measurement

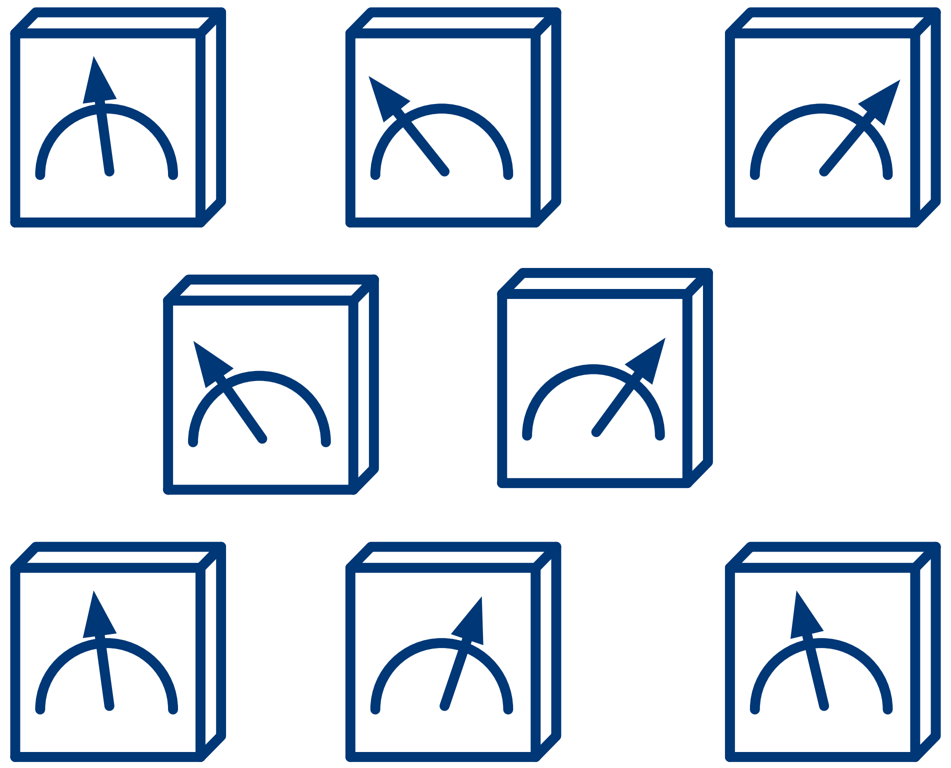
$|\psi\rangle = U|0^n\rangle$

State ρ



Quantum state

$U^\dagger$



Single-qubit Measurement

How to Certify?

- **Approach 0:** Direct measurement

- **Challenge:**

  If we can assume $U^\dagger$ is perfect, then U should be perfect too.

How to Certify?

- **Approach 0:** Direct measurement

- **Challenge:**

  If we can assume $U^\dagger$ is perfect, then U should be perfect too.

  In this world, ρ can be created to be $|\psi\rangle$ perfectly.

How to Certify?

- **Approach 0:** Direct measurement

- **Challenge:**

  If we can assume $U^\dagger$ is perfect, then U should be perfect too.

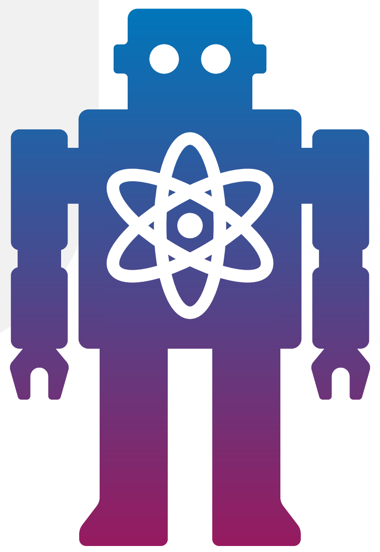
  In this world, ρ can be created to be $|\psi\rangle$ perfectly.

  So we don't need to do any certification.

Question: Simple states

State ρ

External world



- How to certify $|+^n\rangle$?
- How to certify $\dfrac{|0^n\rangle - |1^n\rangle}{\sqrt{2}}$?
- How to certify toric code g.s.?

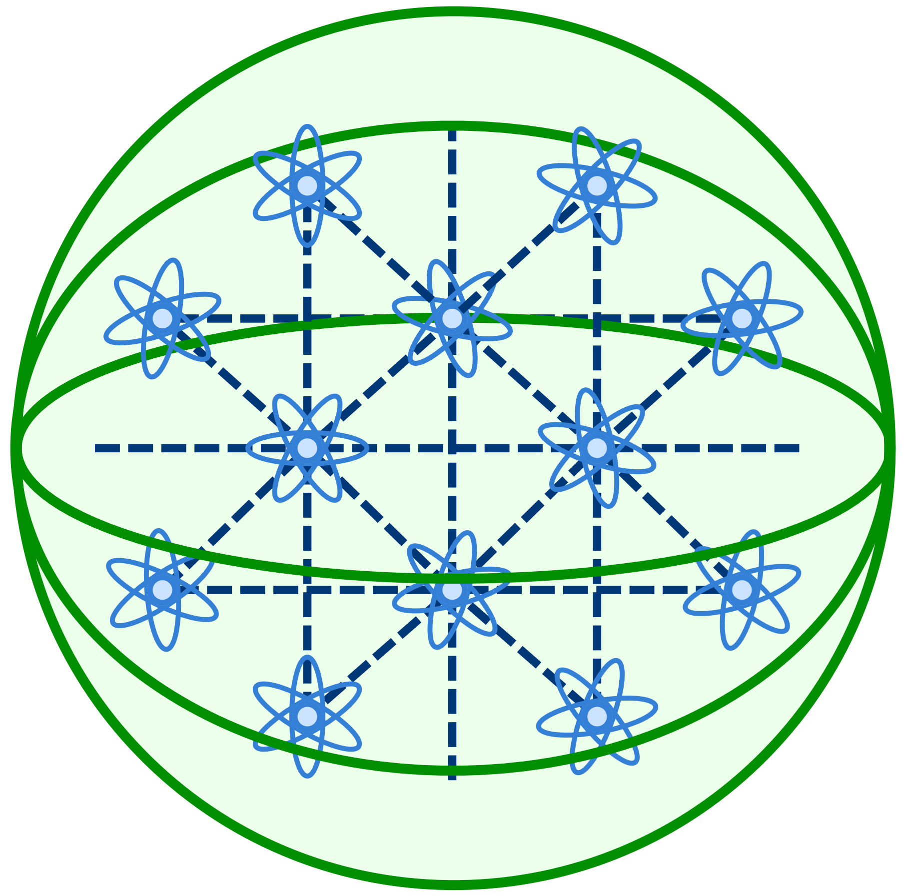
Do it without 2-qubit gates.

How to Certify?

$|\psi\rangle = U|0^n\rangle$

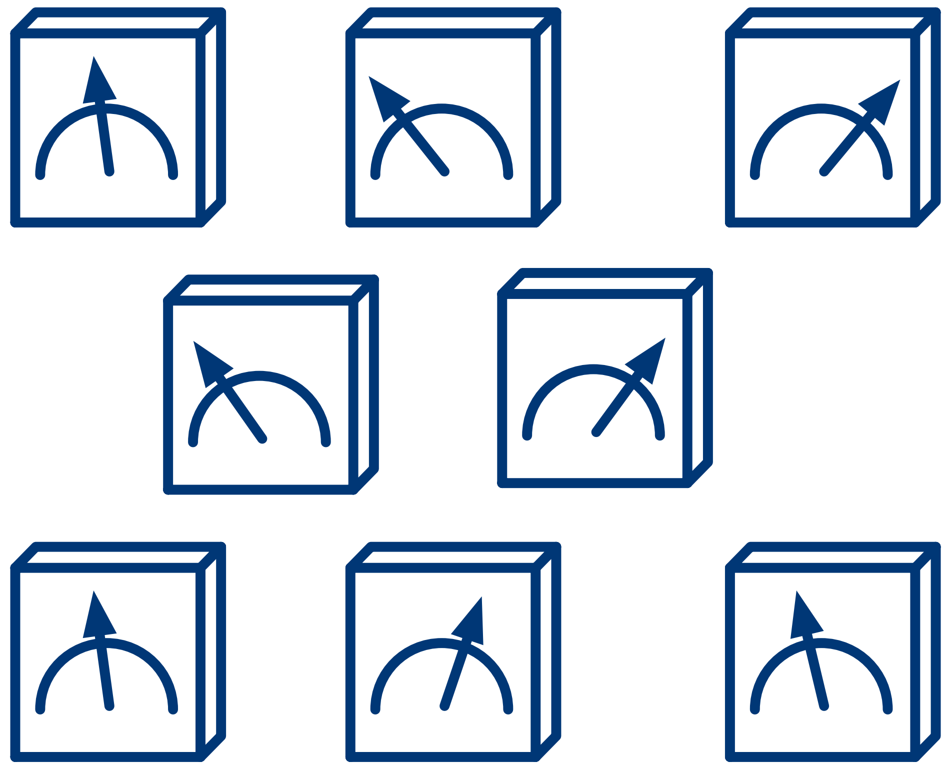
- **Approach 1:** Classical shadow formalism (global 3-design)

State ρ



Quantum state

Random
Clifford Circuit



Single-qubit
Measurement

How to Certify?

$|\psi\rangle = U|0^n\rangle$

- **Approach 1:** Classical shadow formalism (global 3-design)
- **Advantage:**

  Only needs to apply random circuits forming 3-designs on ρ

How to Certify? $|\psi\rangle = U|0^n\rangle$

- **Approach 1:** Classical shadow formalism (global 3-design)
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- **Challenge:**

  Implementing random 3-designs can be **challenging**.

How to Certify?

$|\psi\rangle = U|0^n\rangle$

- **Approach 1:** Classical shadow formalism (global 3-design)

- **Advantage:**

  Only needs to apply random circuits forming 3-designs on ρ

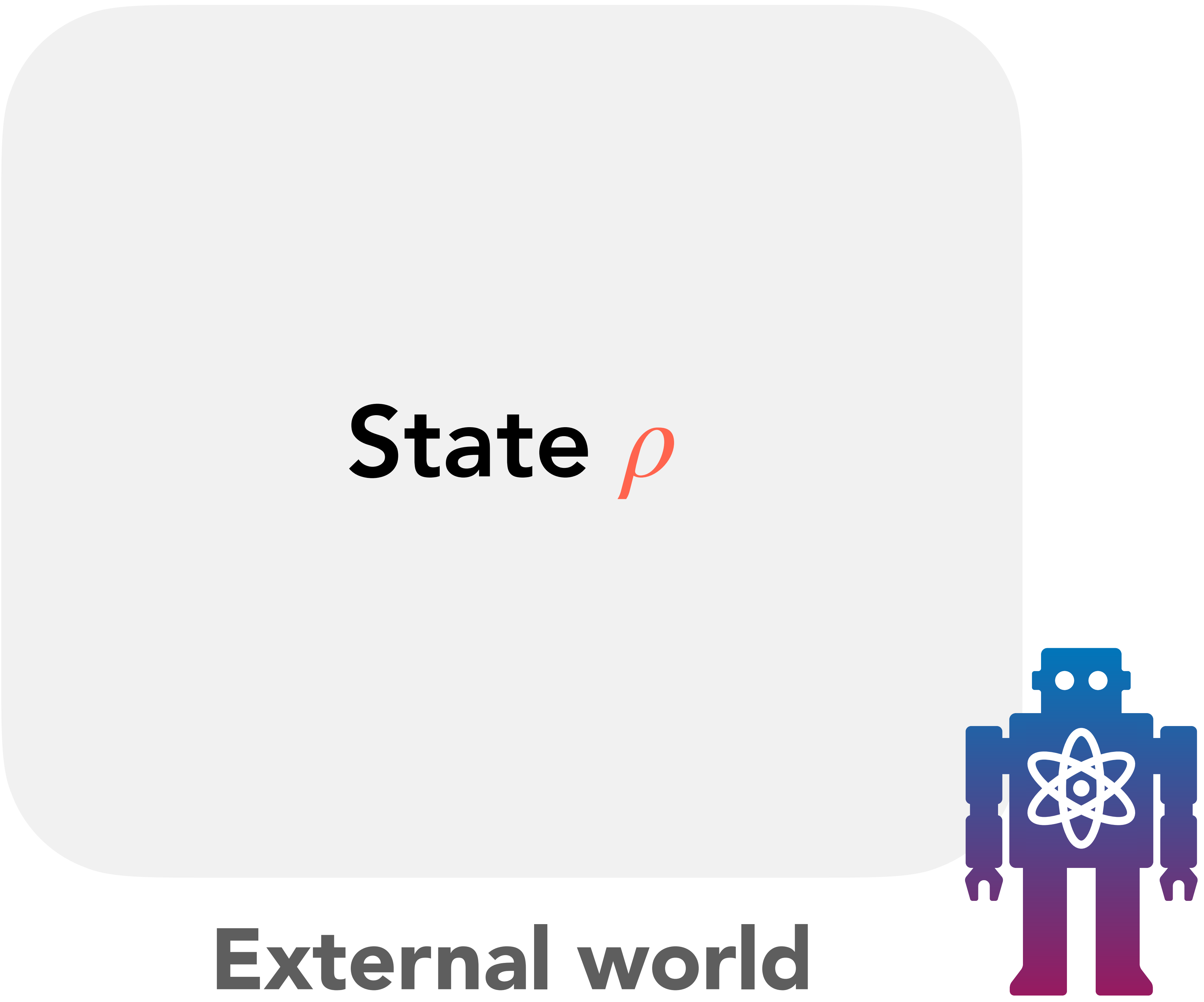
- **Challenge:**

  Implementing random 3-designs can be **challenging**.

  Runtime can be **extremely high** (needs $|\langle s|\psi\rangle|^2$).

  $|s\rangle$ is the single-shot shadow

Question: Any states



How to certify any state $|\psi\rangle$ w/ single-qubit measurements? (non-efficient is ok)

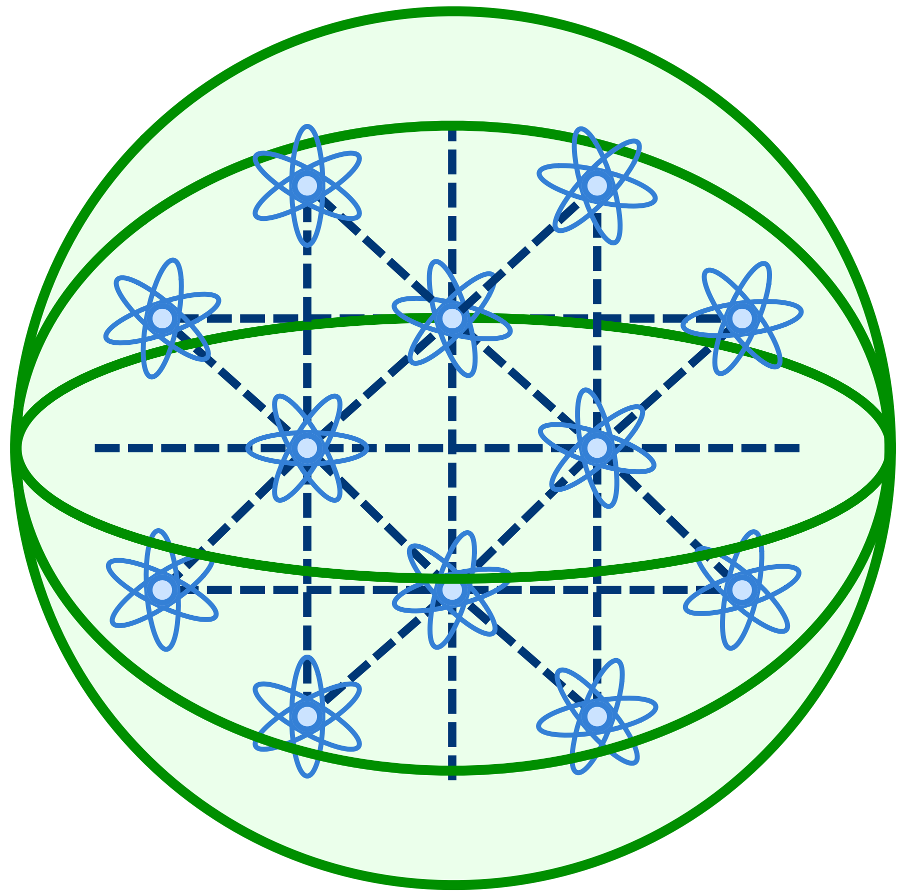
Hint 1: Want to estimate $\mathrm{Tr}(|\psi\rangle\langle\psi|\rho)$.

Hint 2: $|\psi\rangle\langle\psi| = \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} \alpha_P P$.

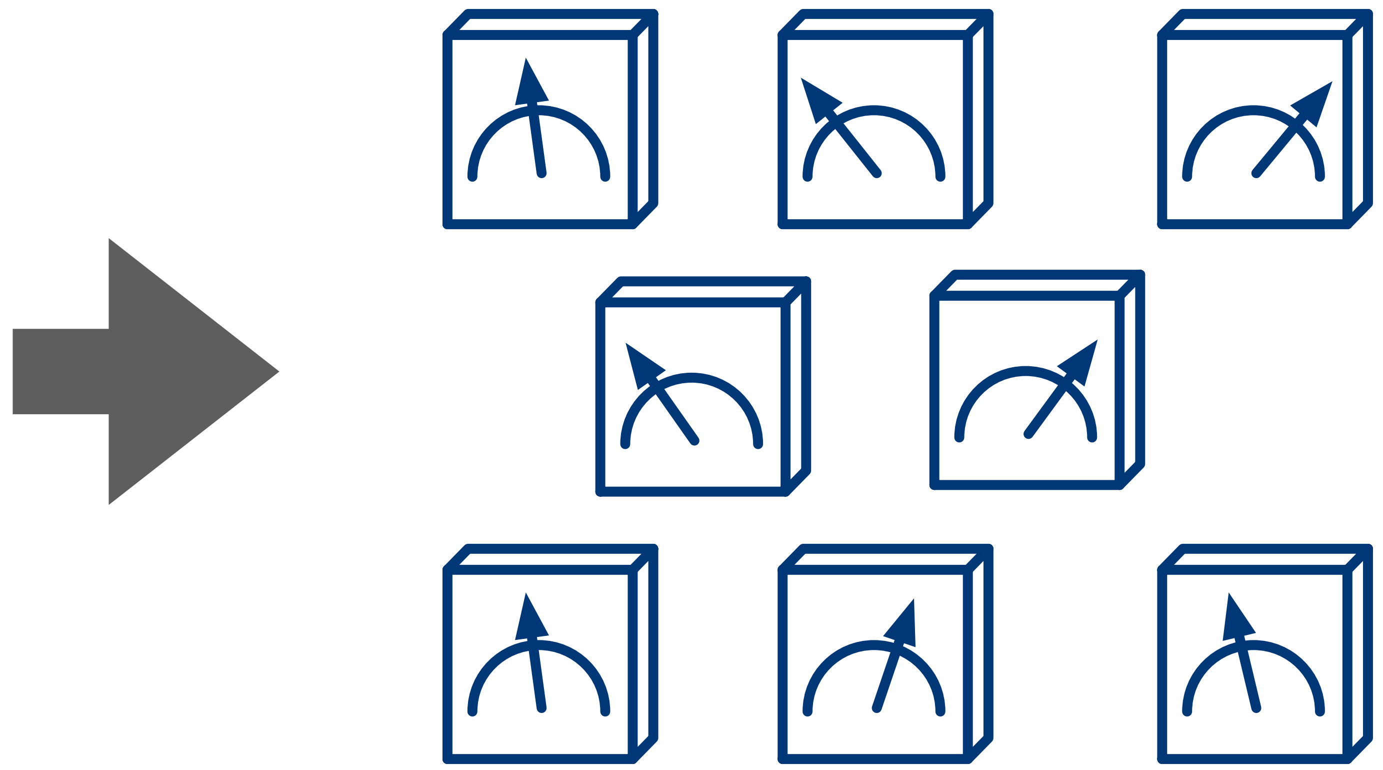
How to Certify? $|\psi\rangle = U|0^n\rangle$

- **Approach 2:** Random Pauli measurements

State ρ



Quantum state



Single-qubit Measurement

How to Certify? $|\psi\rangle = U|0^n\rangle$

- **Approach 2:** Random Pauli measurements
- **Advantage:**

  Only needs **single-qubit** measurements on ρ

How to Certify?

$|\psi\rangle = U|0^n\rangle$

- **Approach 2:** Random Pauli measurements
- **Advantage:**

  Only needs **single-qubit** measurements on ρ
- **Challenge:**

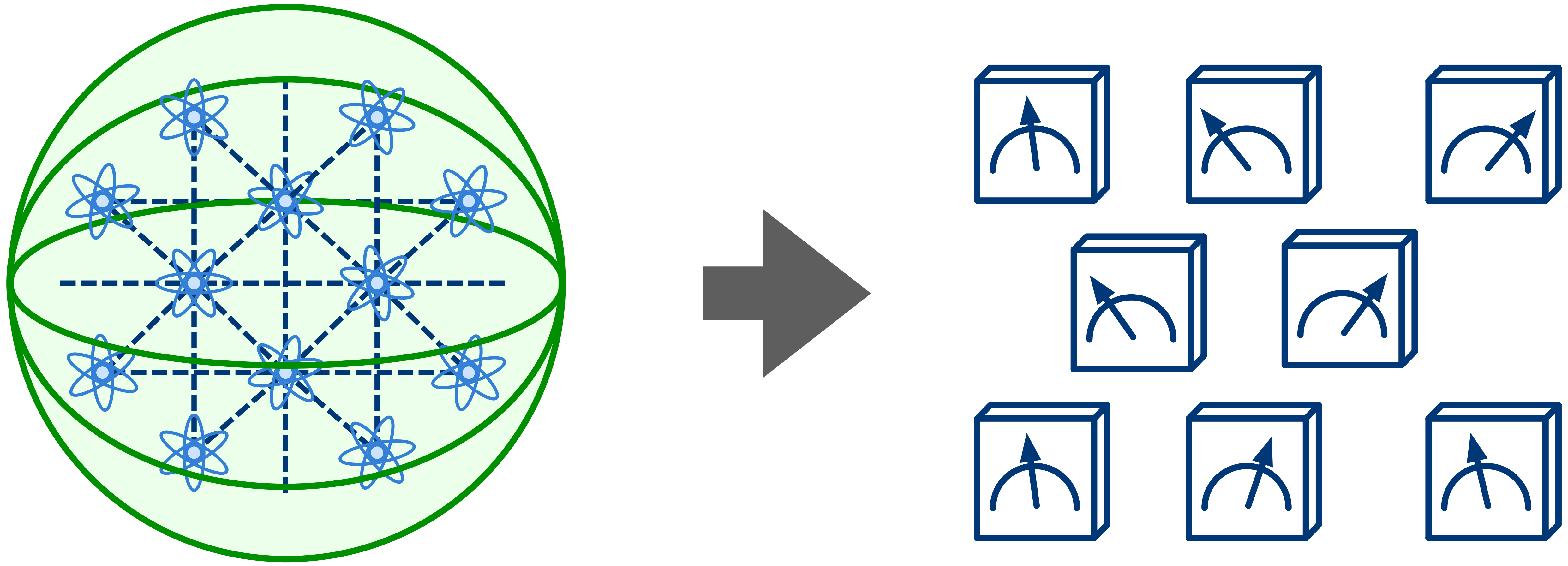
  Requires **exp(n)** measurements for most target $|\psi\rangle$

  especially when $|\psi\rangle$ is highly entangled.

How to Certify? $|\psi\rangle = U|0^n\rangle$

- **Approach 3:** Cross-entropy benchmark $\mathrm{XEB} = \dfrac{2^n \mathbb{E}_{x\sim\langle x|\rho|x\rangle} |\langle x|\psi\rangle|^2 - 1}{2^n \mathbb{E}_{x\sim|\langle x|\psi\rangle|^2} |\langle x|\psi\rangle|^2 - 1},$

State ρ



Quantum state

Single-qubit Measurement (all Z bases)

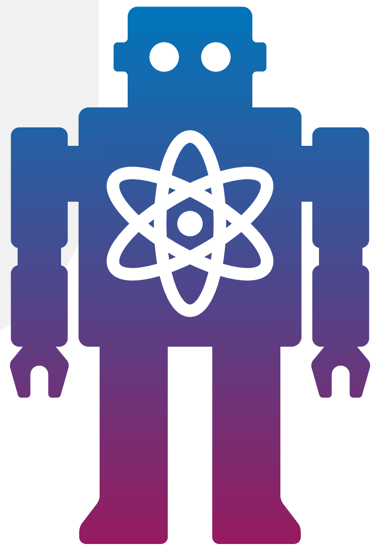
Question: XEB

$|\psi\rangle = U|0^n\rangle$

$$\mathrm{XEB} = \frac{2^n \mathbb{E}_{x \sim \langle x|\rho|x\rangle} |\langle x|\psi\rangle|^2 - 1}{2^n \mathbb{E}_{x \sim |\langle x|\psi\rangle|^2} |\langle x|\psi\rangle|^2 - 1},$$

State ρ

External world



If $\rho \approx (1-p) \cdot |\psi\rangle\langle\psi| + p \cdot \frac{I}{2^n}$,

is XEB a good certifier?

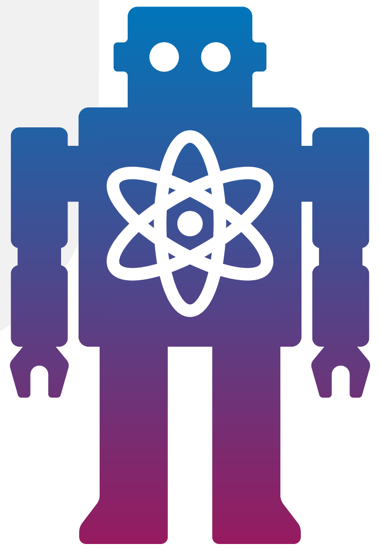
Question: XEB

$|\psi\rangle = U|0^n\rangle$

$$\mathrm{XEB} = \frac{2^n \mathbb{E}_{x\sim\langle x|\rho|x\rangle} |\langle x|\psi\rangle|^2 - 1}{2^n \mathbb{E}_{x\sim|\langle x|\psi\rangle|^2} |\langle x|\psi\rangle|^2 - 1},$$

State ρ

External world

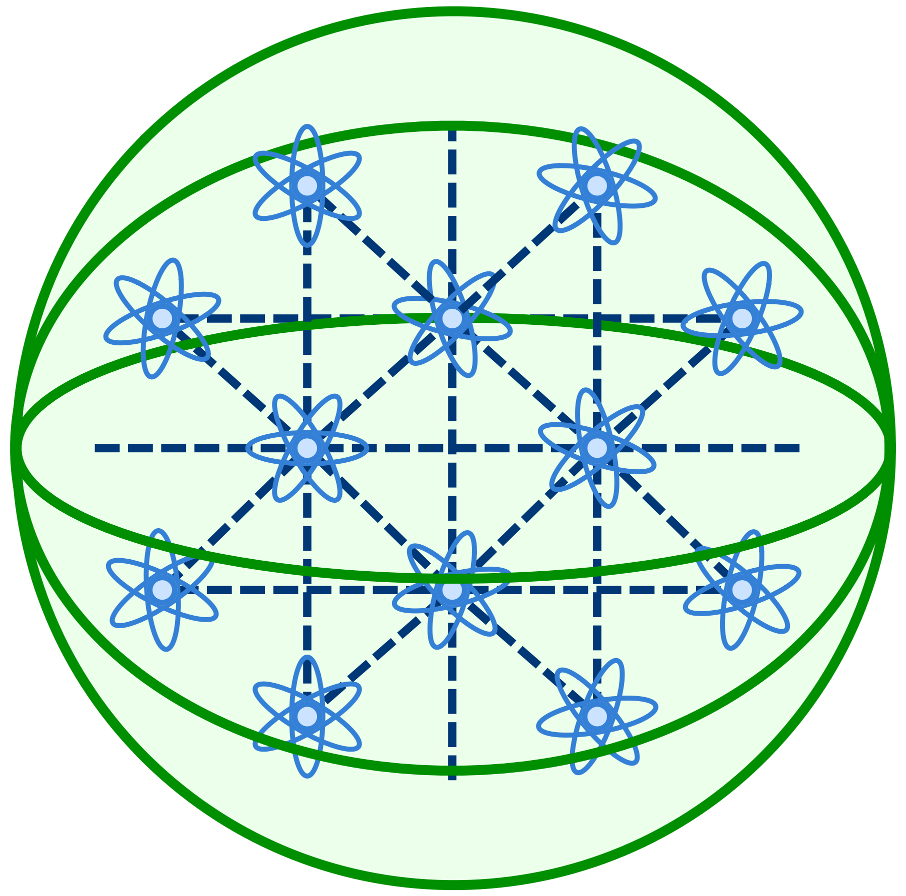


Does there exist ρ and $|\psi\rangle$ such that $\mathrm{XEB} = 1$ and $\langle\psi|\rho|\psi\rangle \approx 0$?

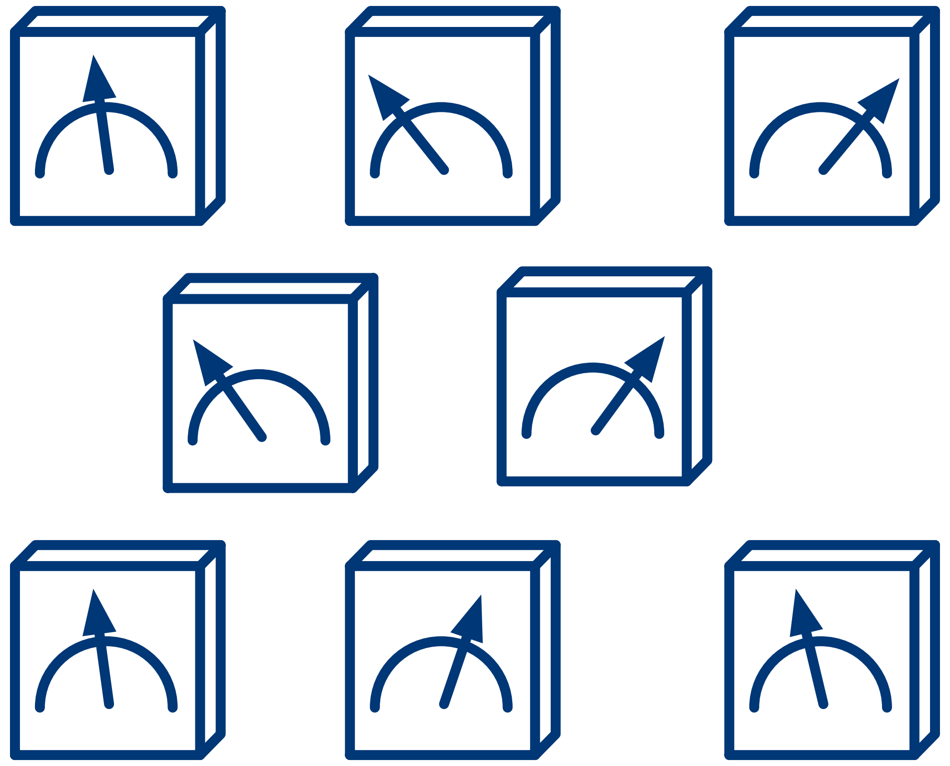
How to Certify? $|\psi\rangle = U|0^n\rangle$

- **Approach 3:** Cross-entropy benchmark $\mathrm{XEB} = \dfrac{2^n \mathbb{E}_{x\sim\langle x|\rho|x\rangle} |\langle x|\psi\rangle|^2 - 1}{2^n \mathbb{E}_{x\sim|\langle x|\psi\rangle|^2} |\langle x|\psi\rangle|^2 - 1},$

State ρ



Quantum state



Single-qubit Measurement (all Z bases)

How to Certify?

- **Approach 3:** Cross-entropy benchmark (XEB)
- **Advantage:**

  Only needs single-qubit measurements (Z-basis) on ρ

How to Certify?

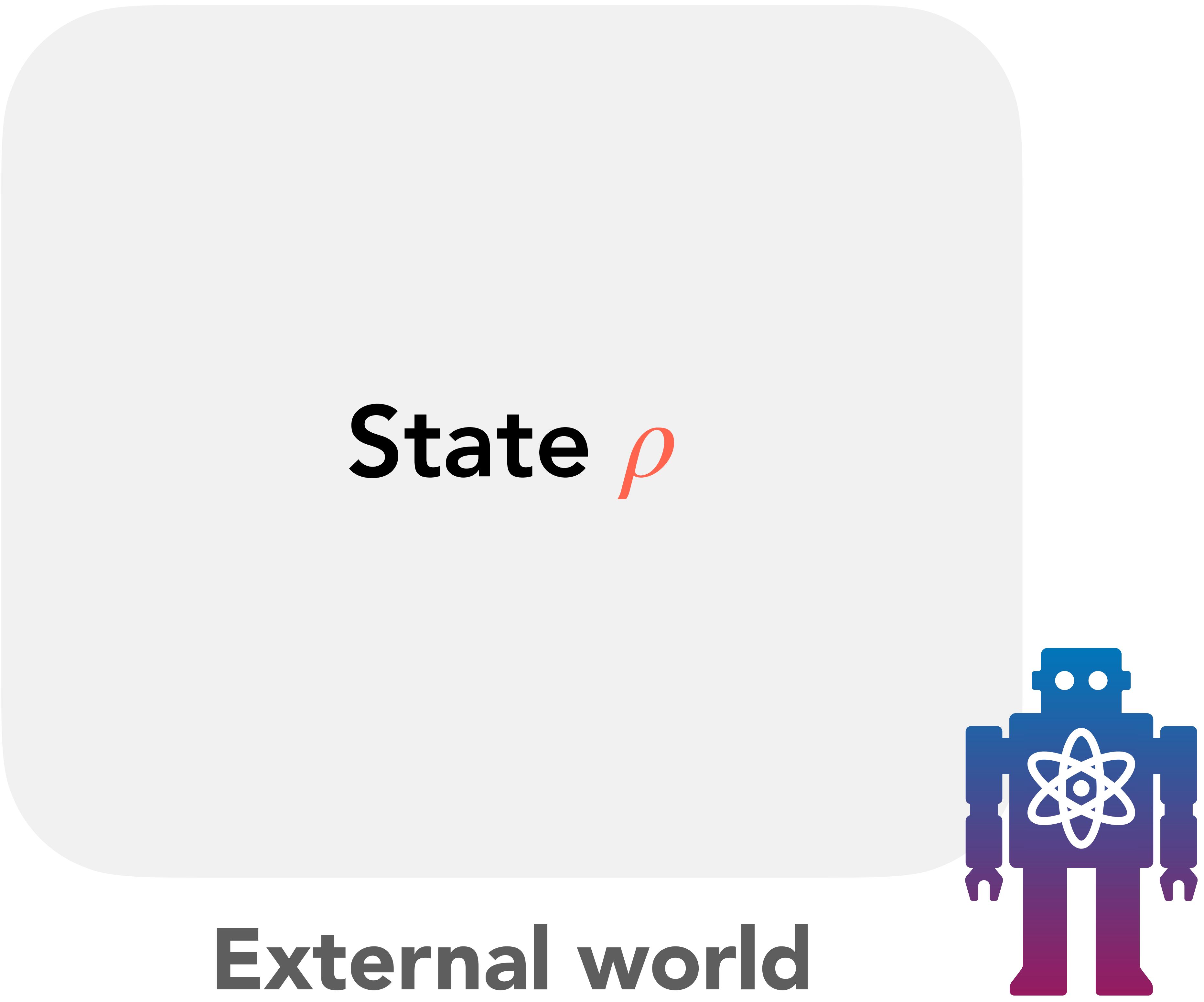
- **Approach 3:** Cross-entropy benchmark (XEB)
- **Advantage:**

  Only needs **single-qubit** measurements (Z-basis) on ρ
- **Challenge:**

  Does not rigorously address the certification task.

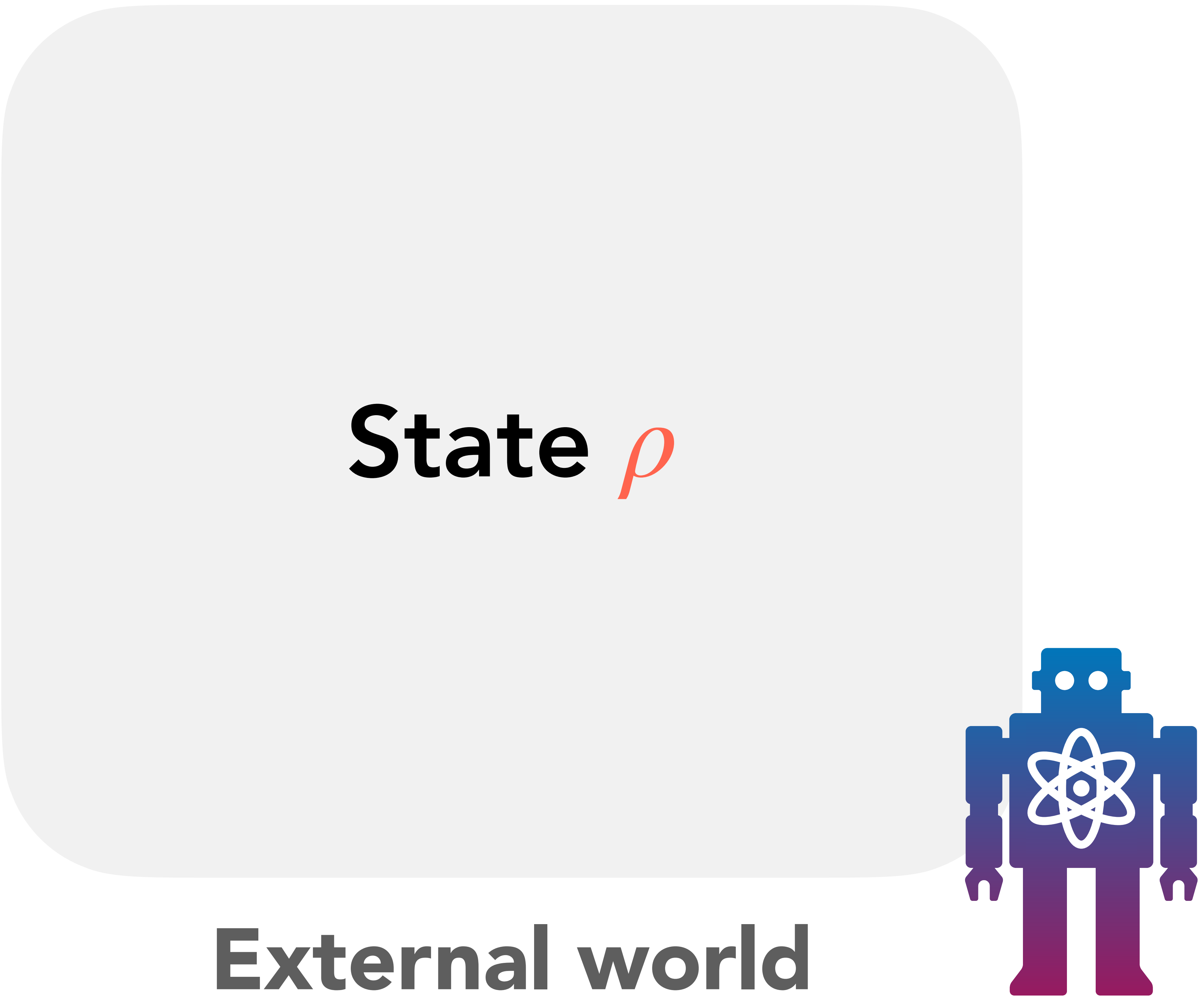
  ρ can be **far** from $|\psi\rangle\langle\psi|$ despite perfect XEB score.

Question: Generic State



Can XEB be used to certify **almost any** state $|\psi\rangle$ w/ few single-qubit measurements?

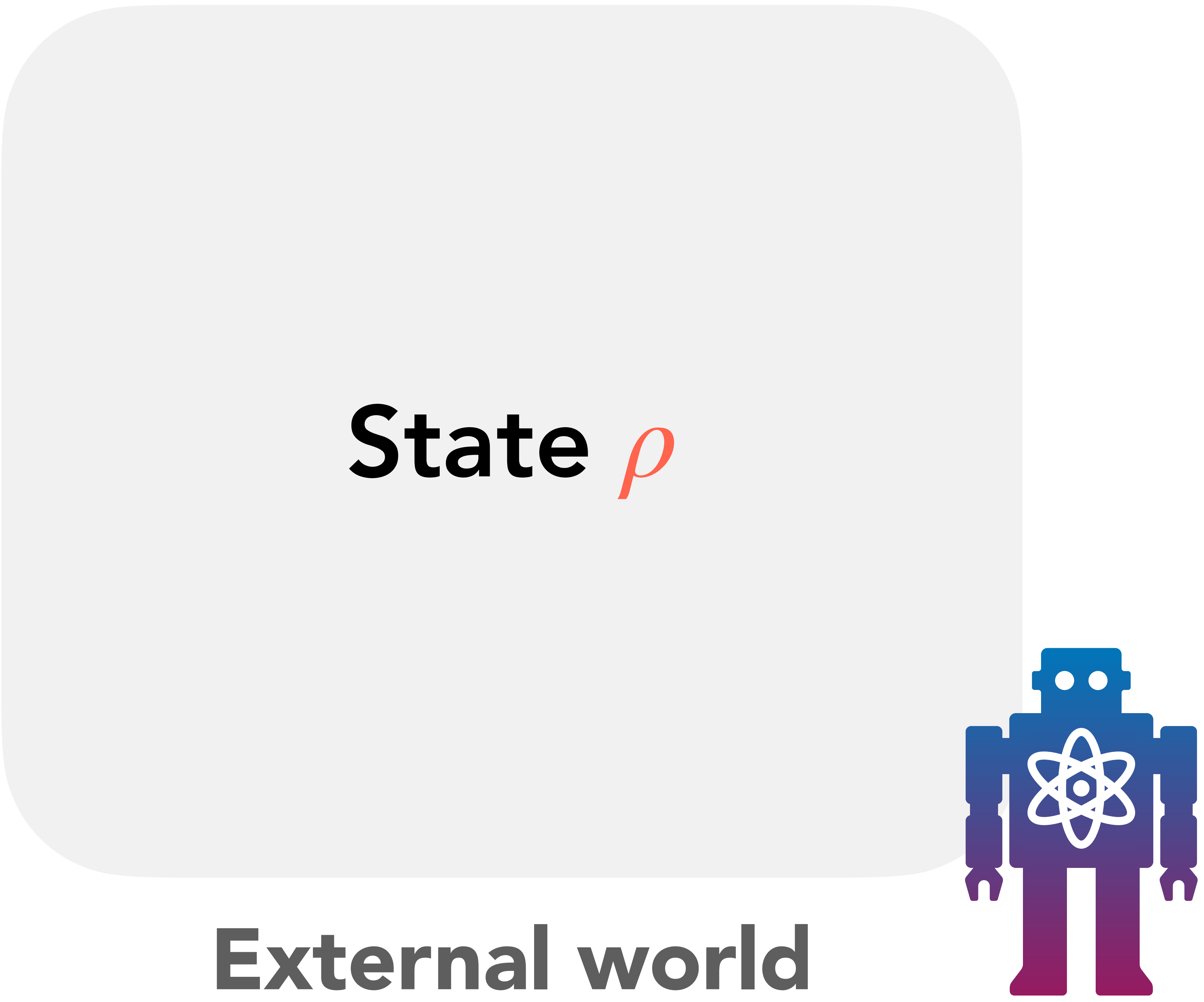
Question: Generic State



Can XEB be used to certify **almost any** state $|\psi\rangle$ w/ few single-qubit measurements?

Hint 1: No.

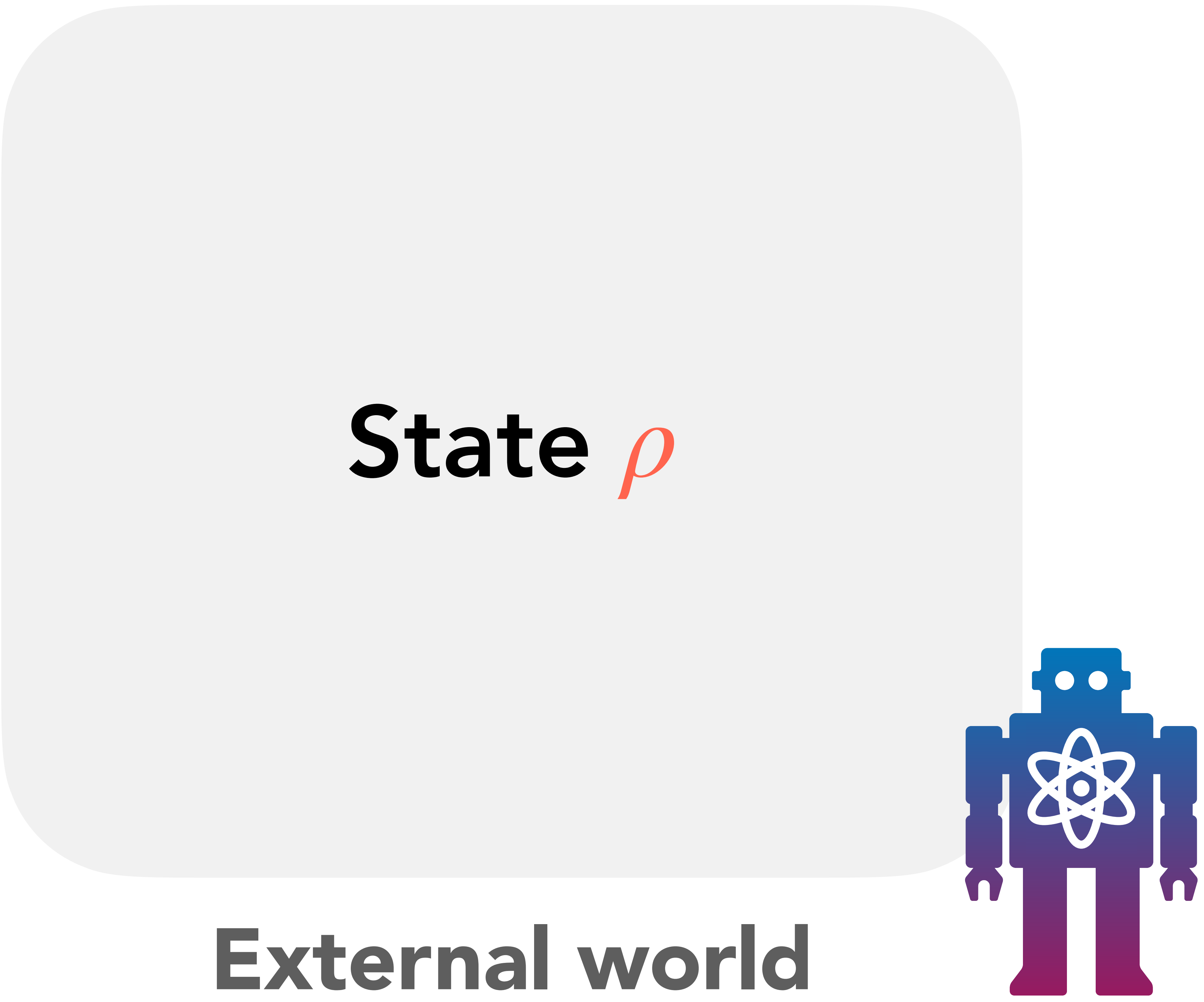
Question: Generic State



Can XEB be used to certify **almost any** state $|\psi\rangle$ w/ few single-qubit measurements?

Hint 1: No.
Hint 2: Dephasing noise.

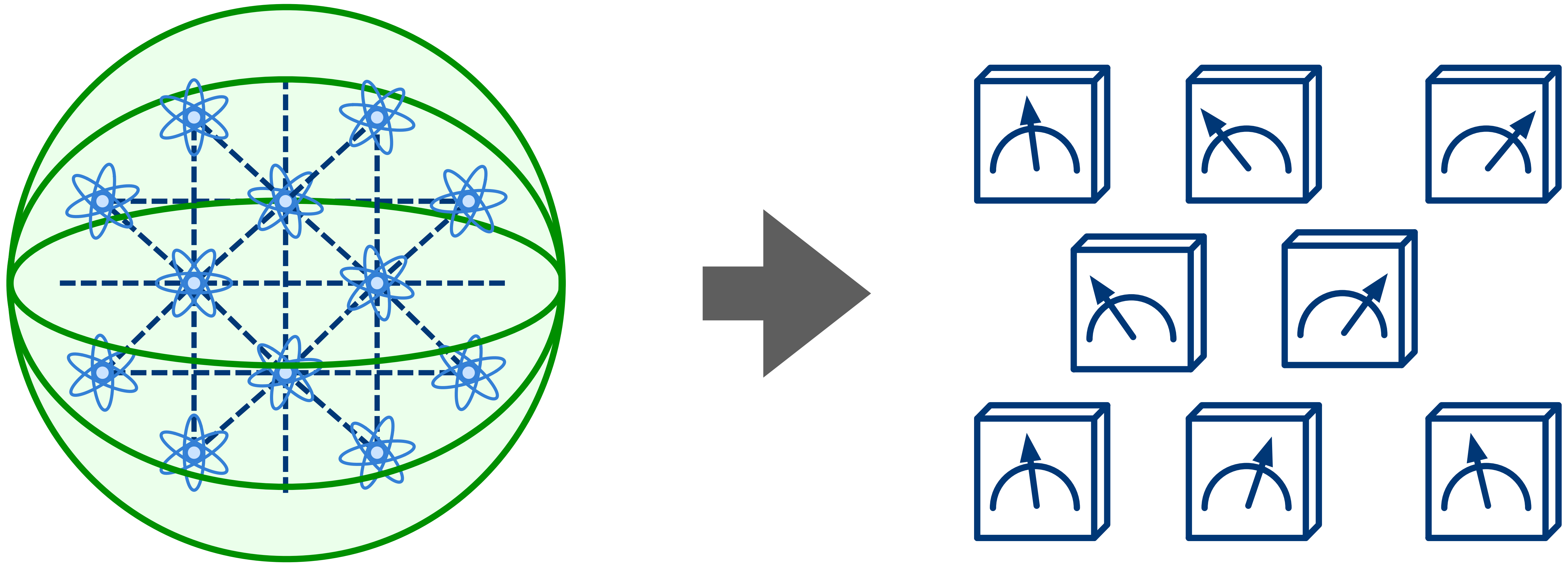
Question: Generic and Rigorous



Can we certify **almost any** state $|\psi\rangle$ w/ few single-qubit measurements?

Measurement Protocol

- Repeat the following measurement a few times.

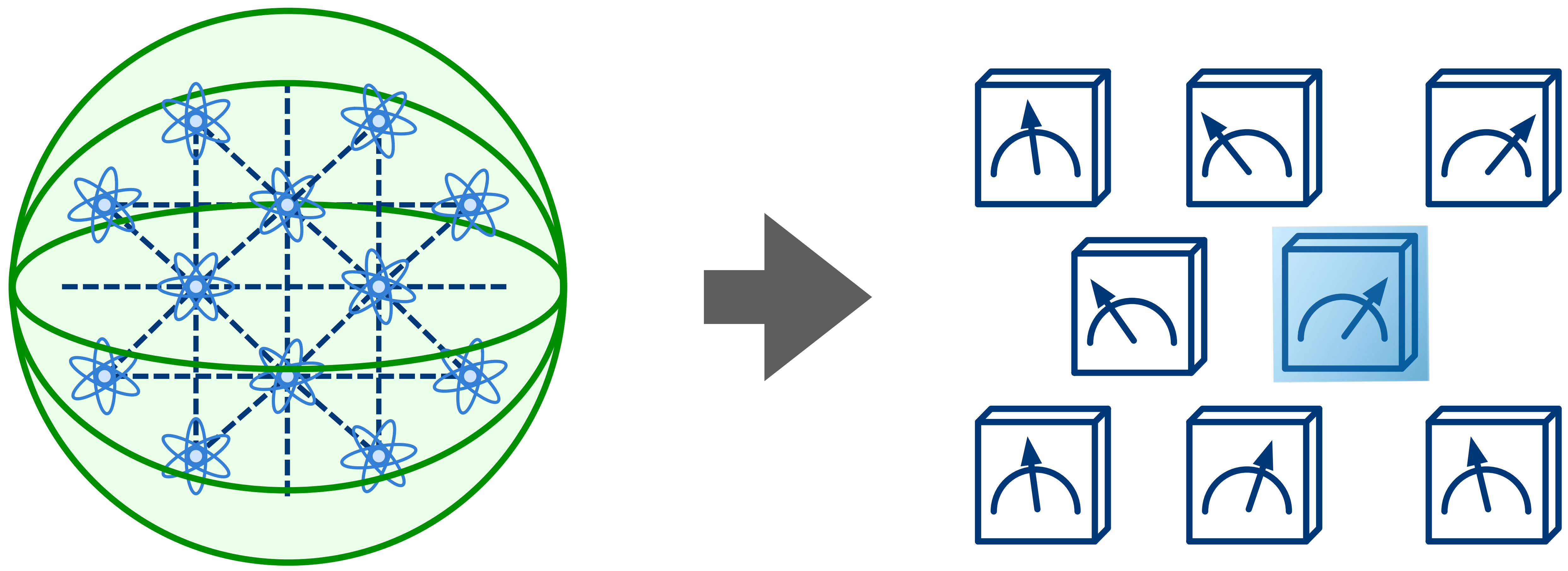


Quantum state

Single-qubit Measurement

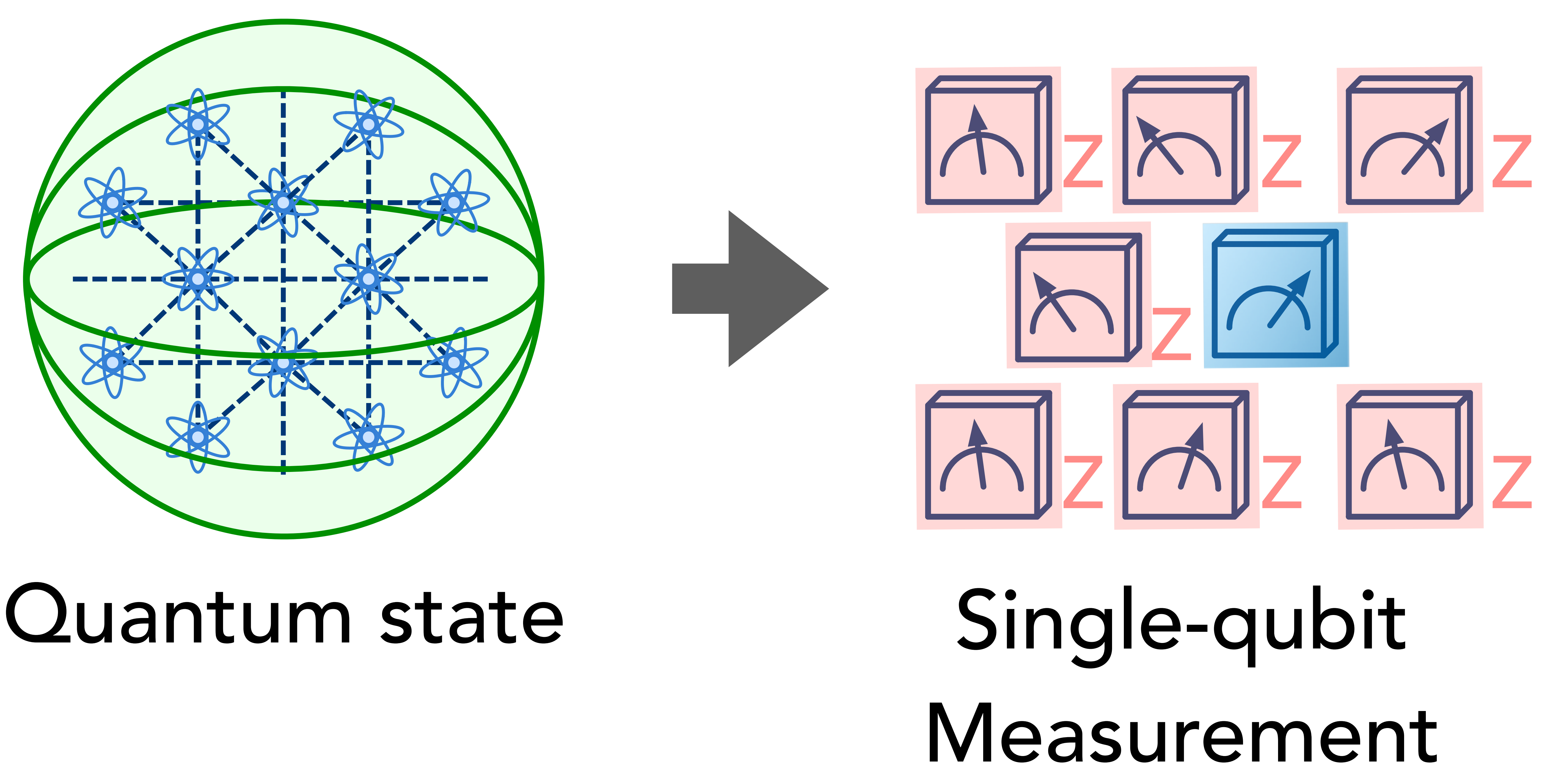
Measurement Protocol

- Pick a random qubit x.



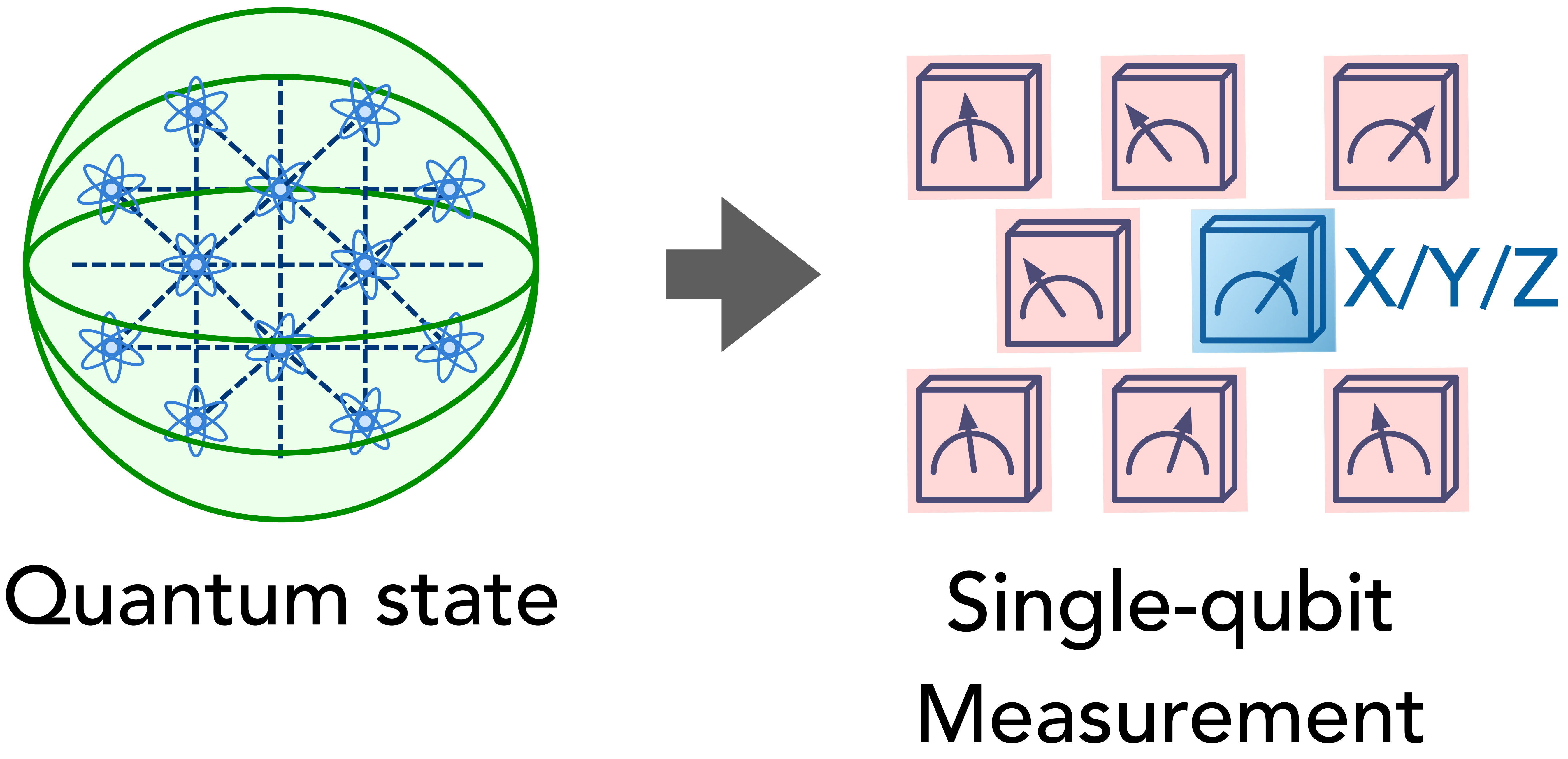
Measurement Protocol

- Pick a random qubit x. Measure all except qubit x in Z basis.



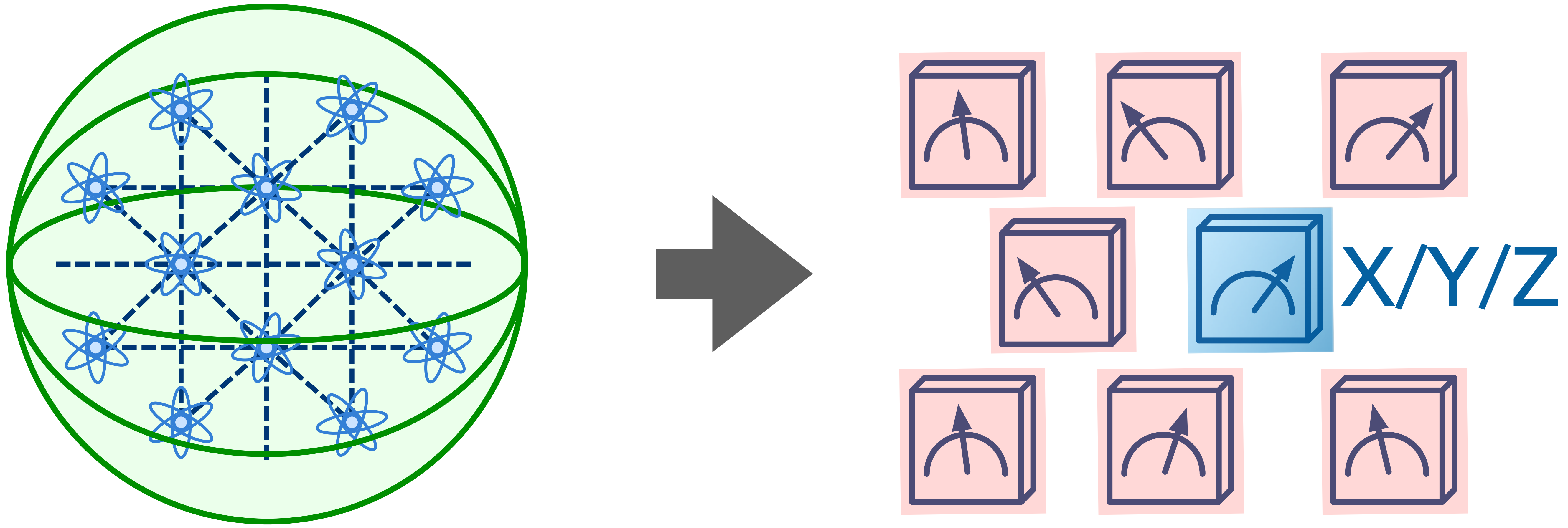
Measurement Protocol

- Pick a random qubit x. Measure x in random X/Y/Z basis.



Measurement Protocol

- That's it.



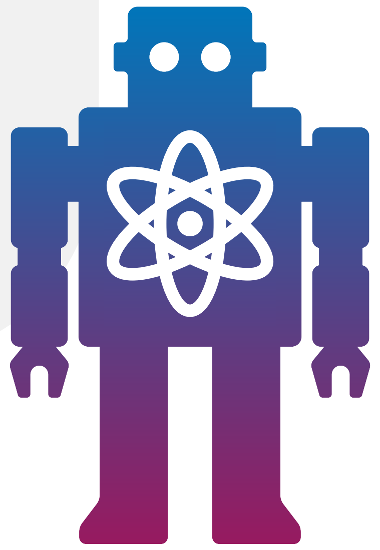
Quantum state

Single-qubit Measurement

Question: Sufficiency

State ρ

External world

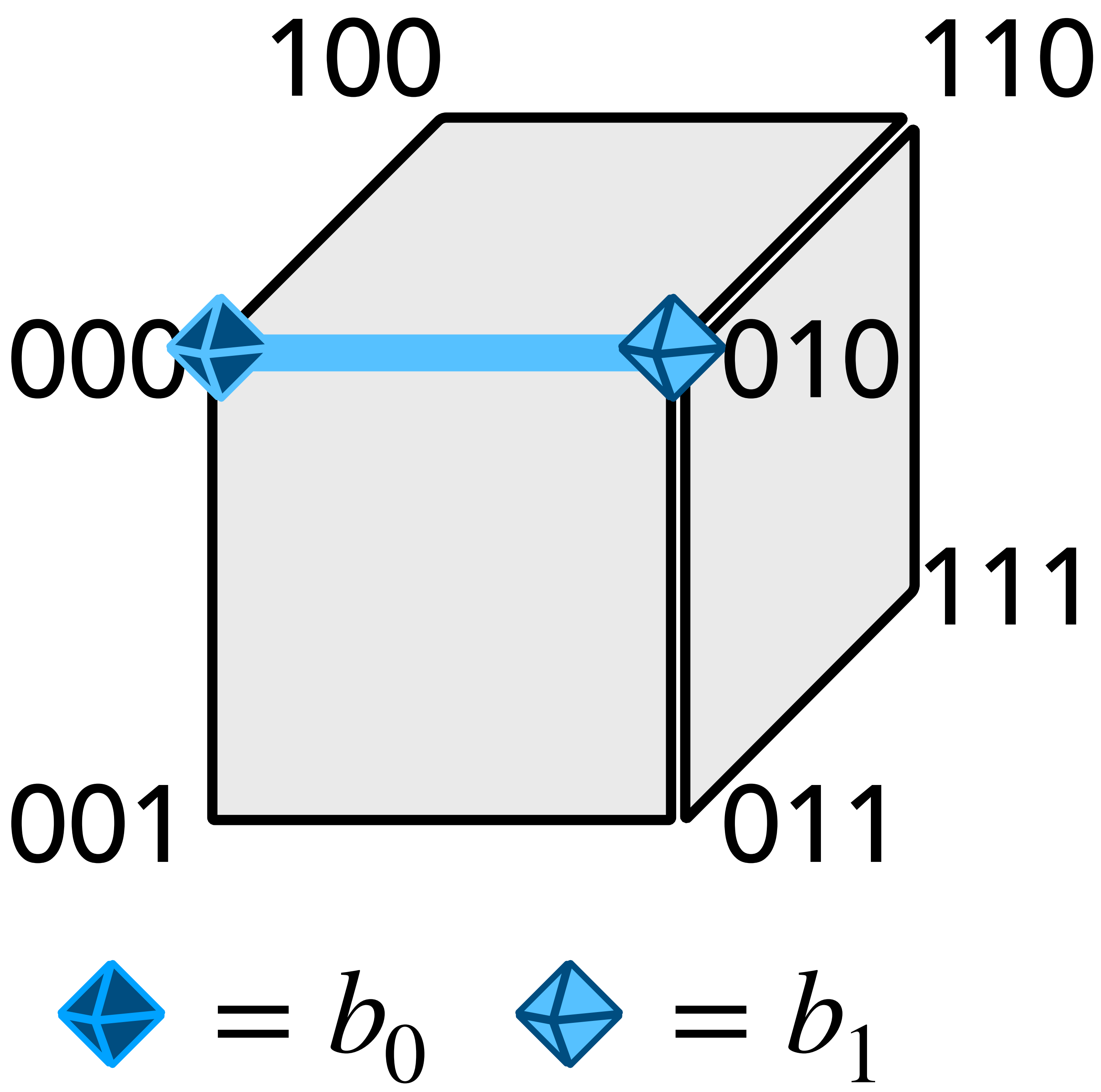


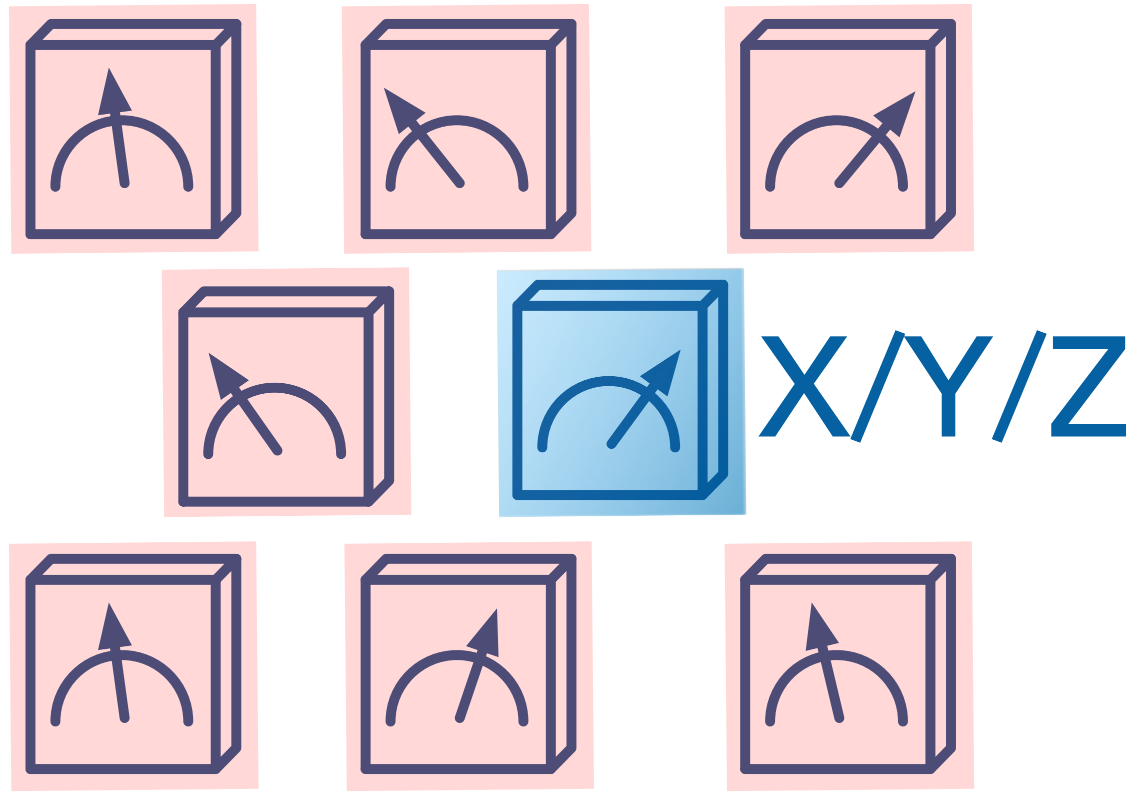
Is the measurement data **sufficient** to certify:

- $|0^n\rangle$ or $|+^n\rangle$?
- any product state?
- any $\frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle$?

Postprocessing

- The measurement outcomes on  specifies two bitstrings (b_0, b_1) that differ by exactly one bit.

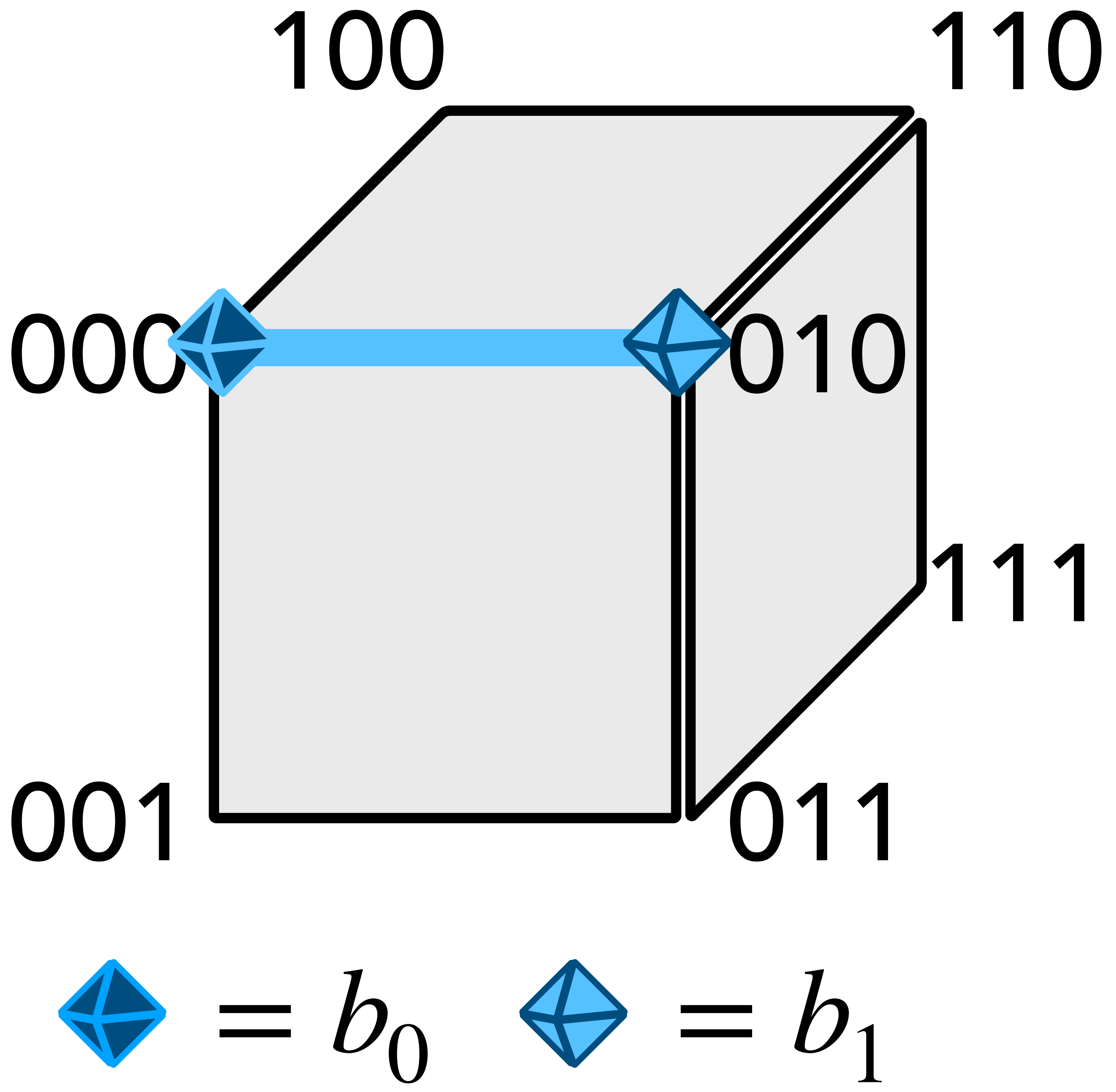


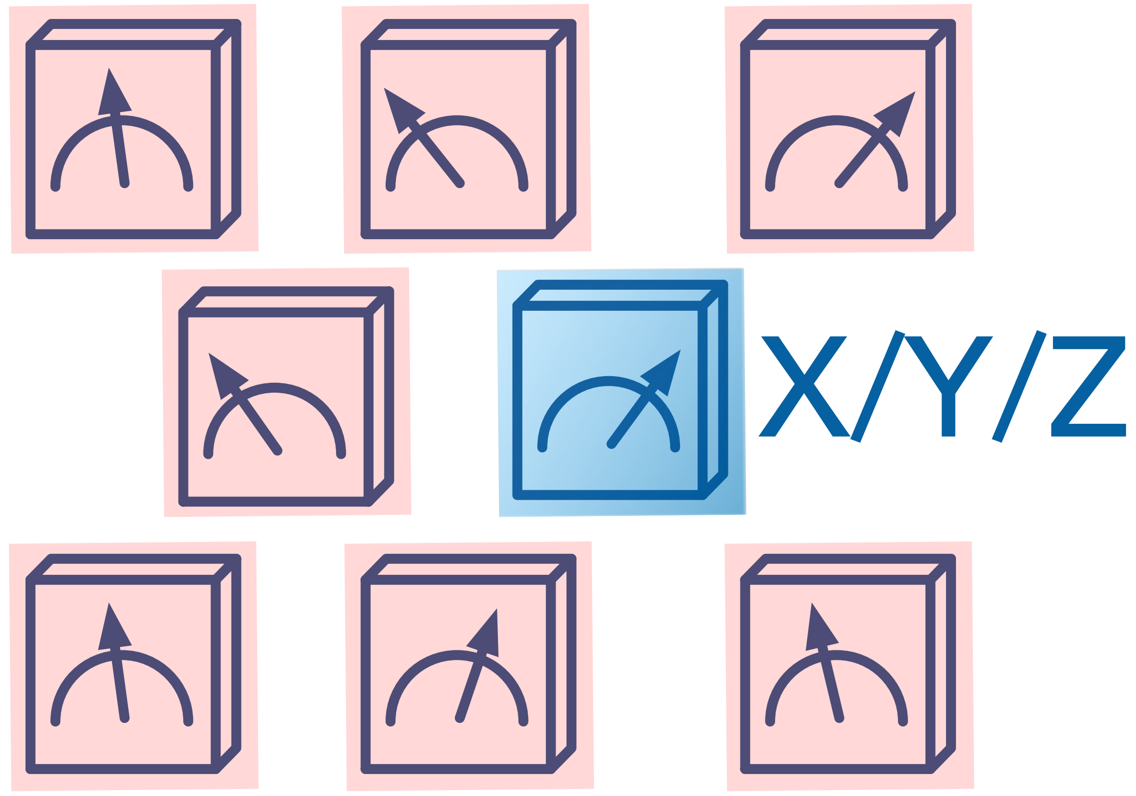


Single-qubit Measurement

Postprocessing

- The **ideal** post-measurement 1-qubit state $|\psi_{b_0,b_1}\rangle$ on **qubit** x is proportional to $\langle b_0|\psi\rangle|0\rangle + \langle b_1|\psi\rangle|1\rangle$.

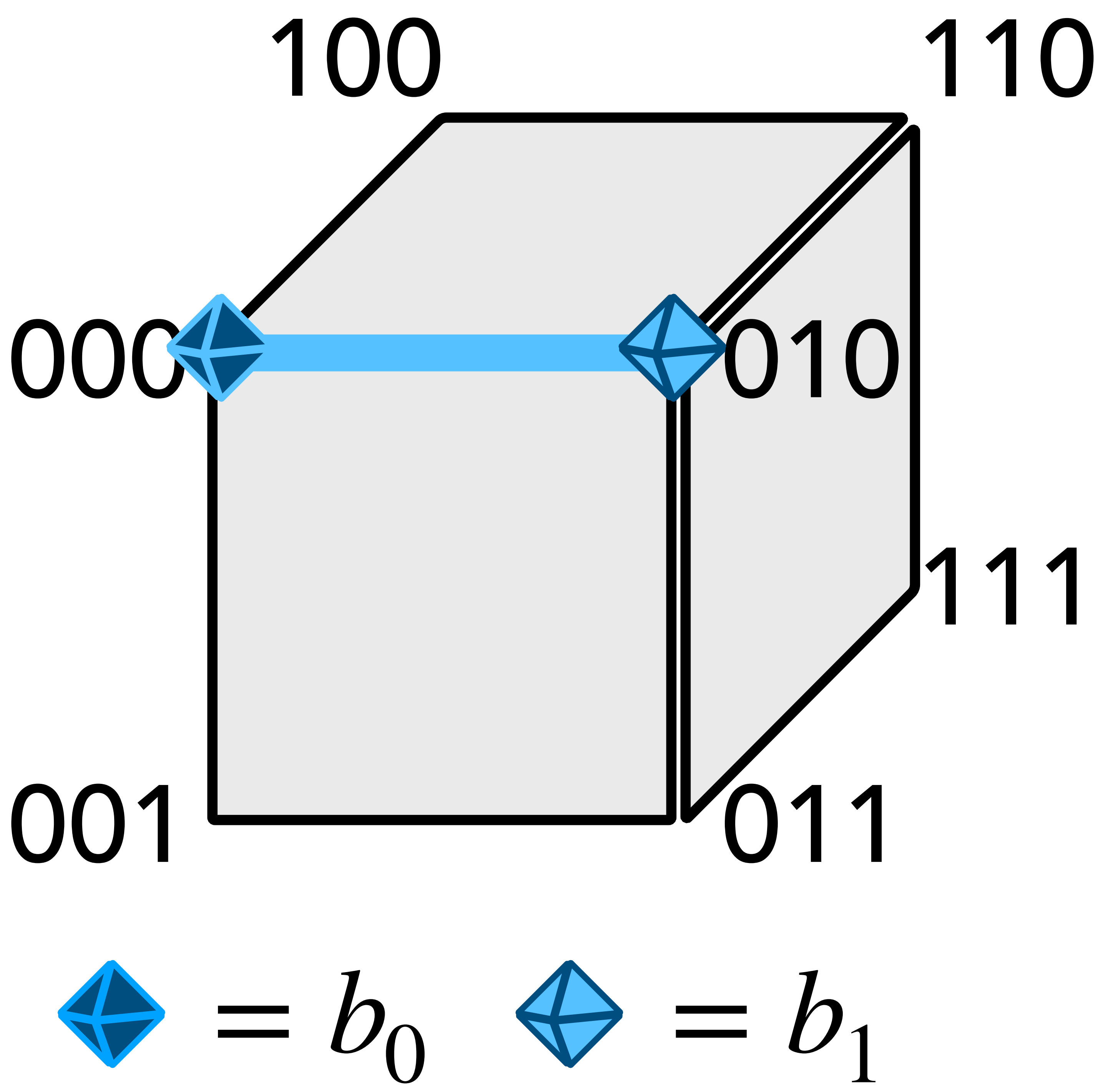


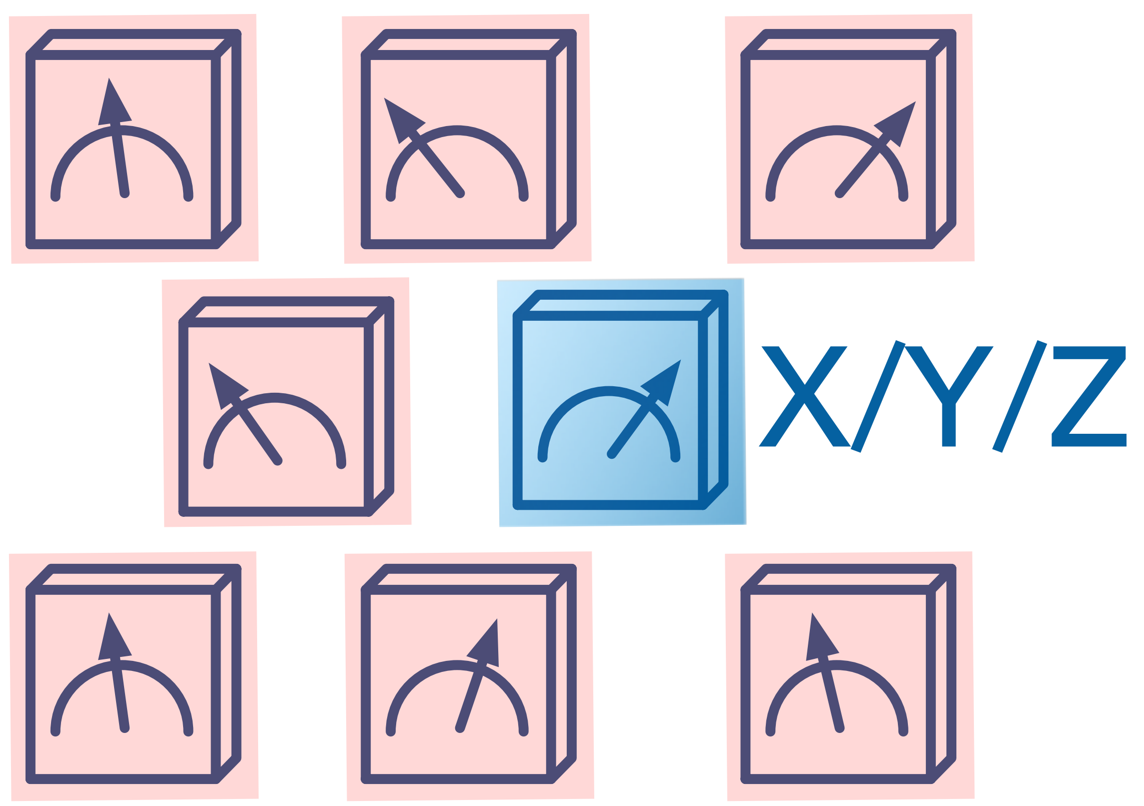


Single-qubit Measurement

Postprocessing

- Use randomized Pauli measurement (classical shadow) on **qubit** x to predict the fidelity ω with the **ideal** 1-qubit state $|\psi_{b_0,b_1}\rangle$.





Single-qubit Measurement

Postprocessing

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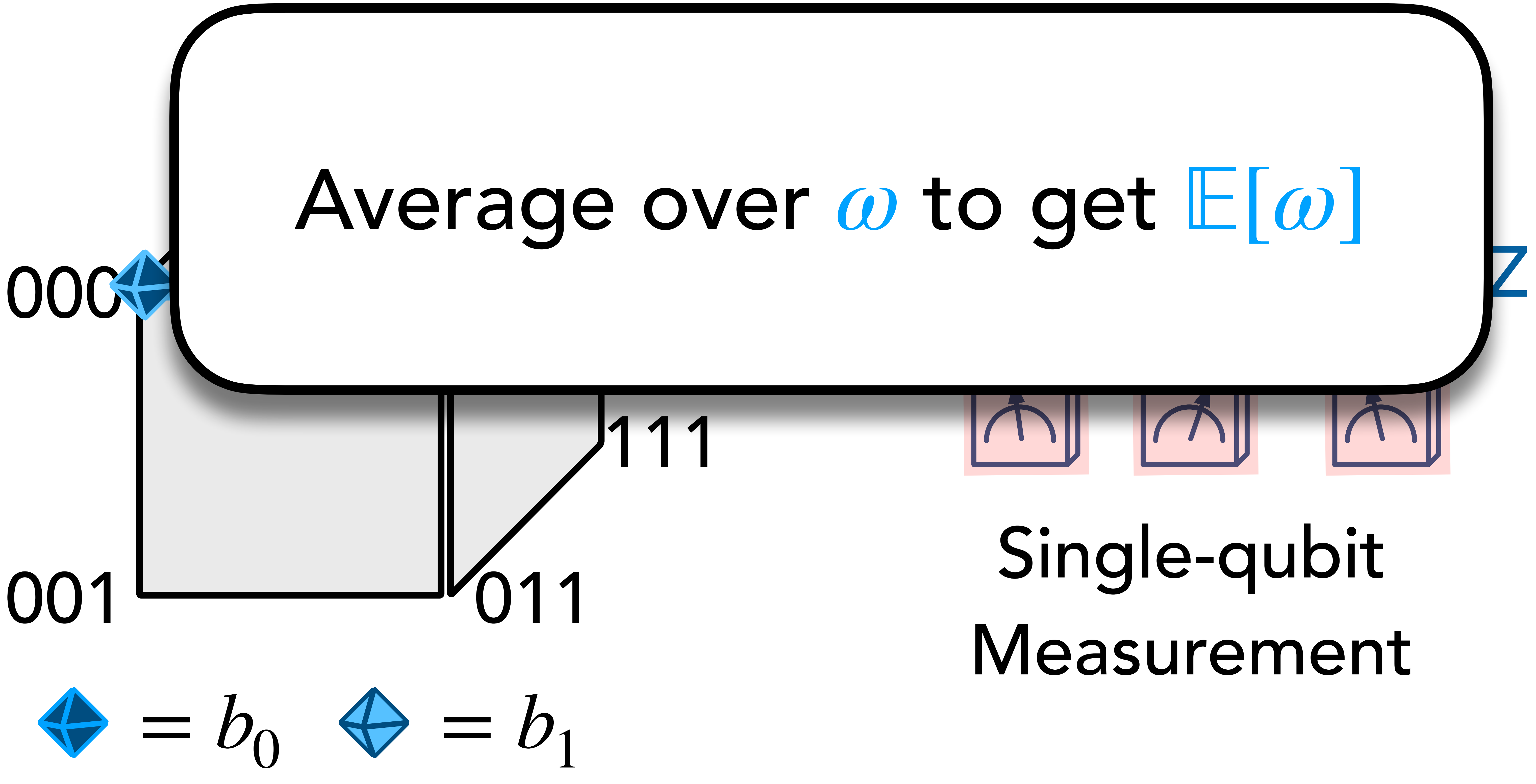
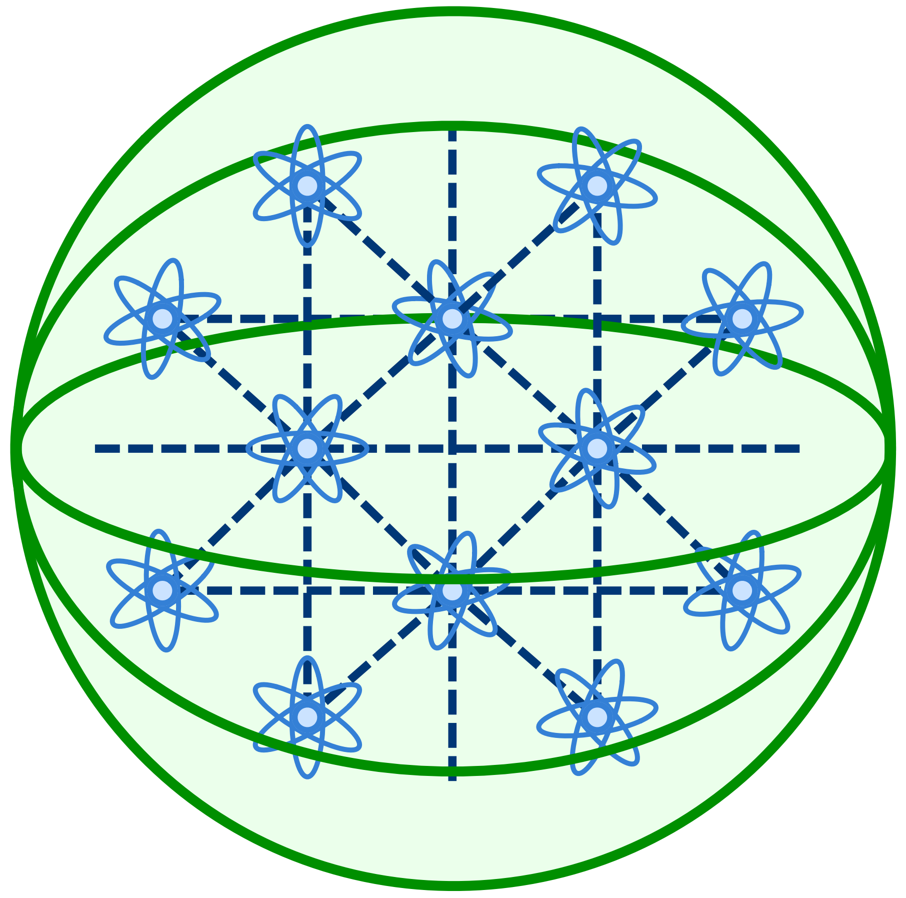


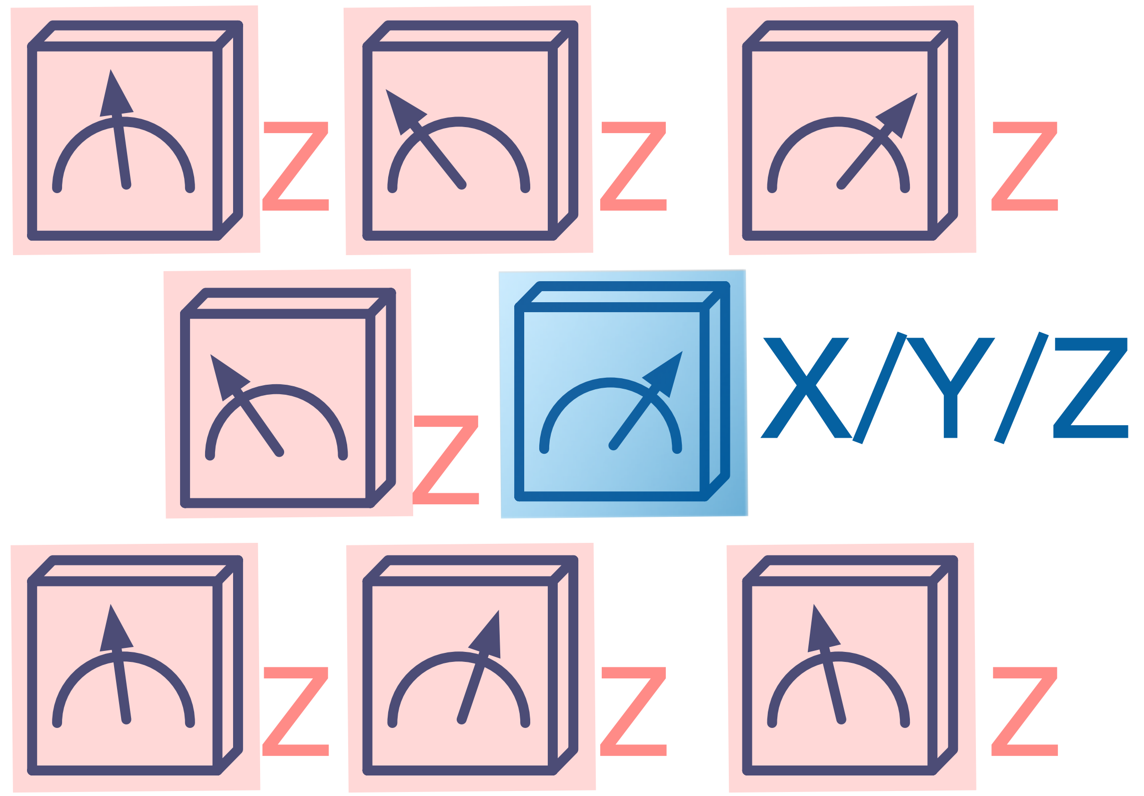
Question: Shadow Overlap

What is the **analytical form** of $\mathbb{E}[\omega]$?

ω is an estimator for the fidelity with the **ideal** 1-qubit state $|\psi_{b_0,b_1}\rangle$



Quantum state



Single-qubit Measurement

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$$\mathbb{E}[\omega] = \frac{1}{n}\sum_{i=1}^{n}\sum_{b_{\neq i}\in\{0,1\}^{n-1}} \mathrm{Tr}\left(\langle b_{\neq i}|\rho|b_{\neq i}\rangle \frac{\langle b_{\neq i}|\psi\rangle\langle\psi|b_{\neq i}\rangle}{\mathrm{Tr}\langle b_{\neq i}|\psi\rangle\langle\psi|b_{\neq i}\rangle}\right)$$

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$$= \mathrm{Tr}\left(L_{|\psi\rangle}\cdot\rho\right) \in [0,1]$$

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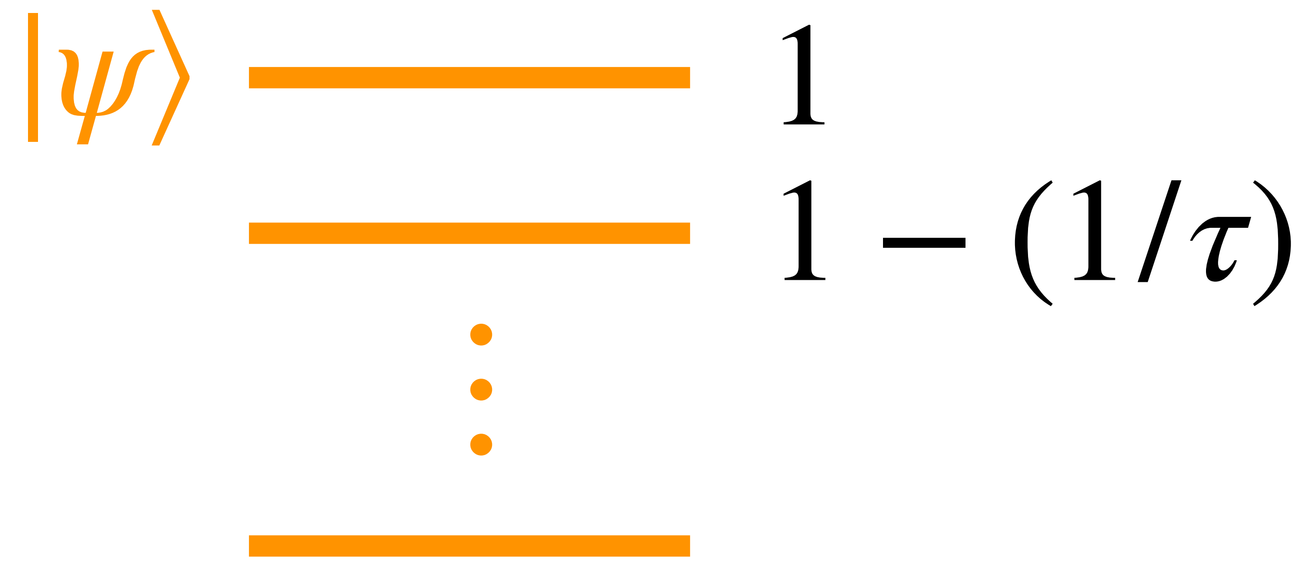
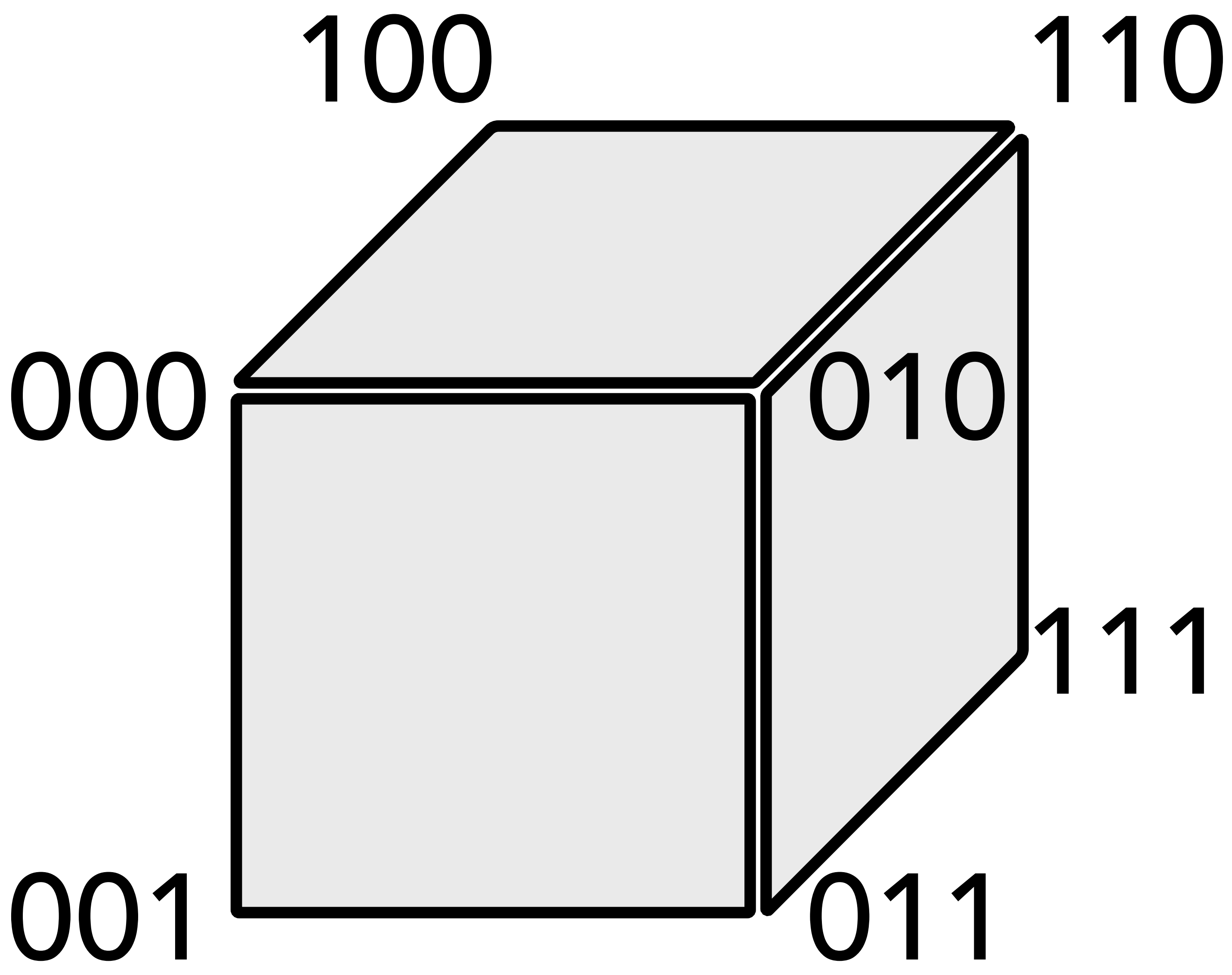


Spectrum of $L_{|\psi\rangle}$

Relaxation Time

- Consider an n-qubit target state $|\psi\rangle$.
- Choose a basis $|b\rangle$, where $b \in \{0,1\}^n$ is a bitstring.
- Let $\pi(b) = |\langle b|\psi\rangle|^2$ be the **measurement distribution**.

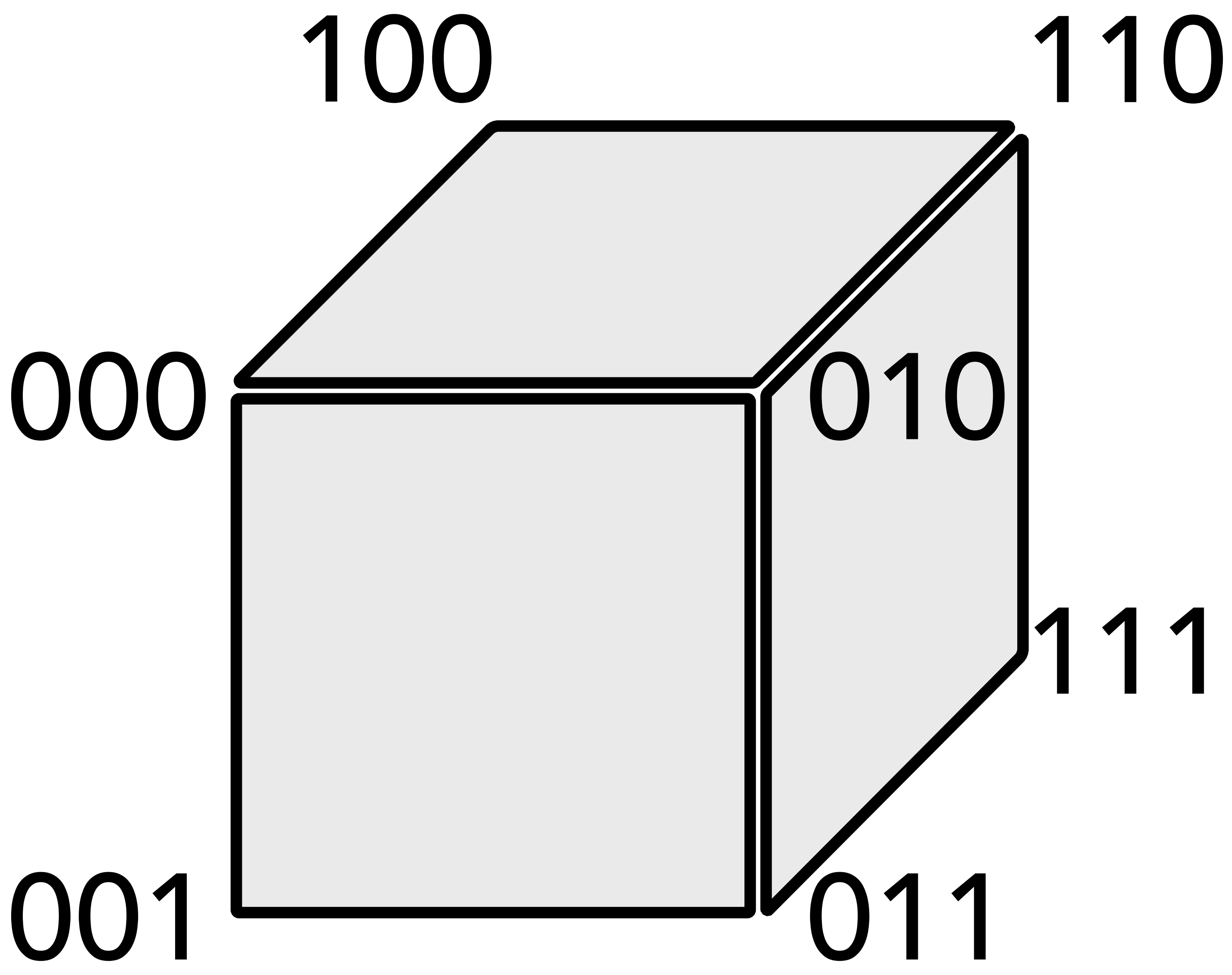
Boolean
Hypercube



Relaxation Time

- Let $\pi(b) = |\langle b|\psi\rangle|^2$ be the **measurement distribution**.
- Consider a random walk on n-bit Boolean hypercube.

Boolean
Hypercube



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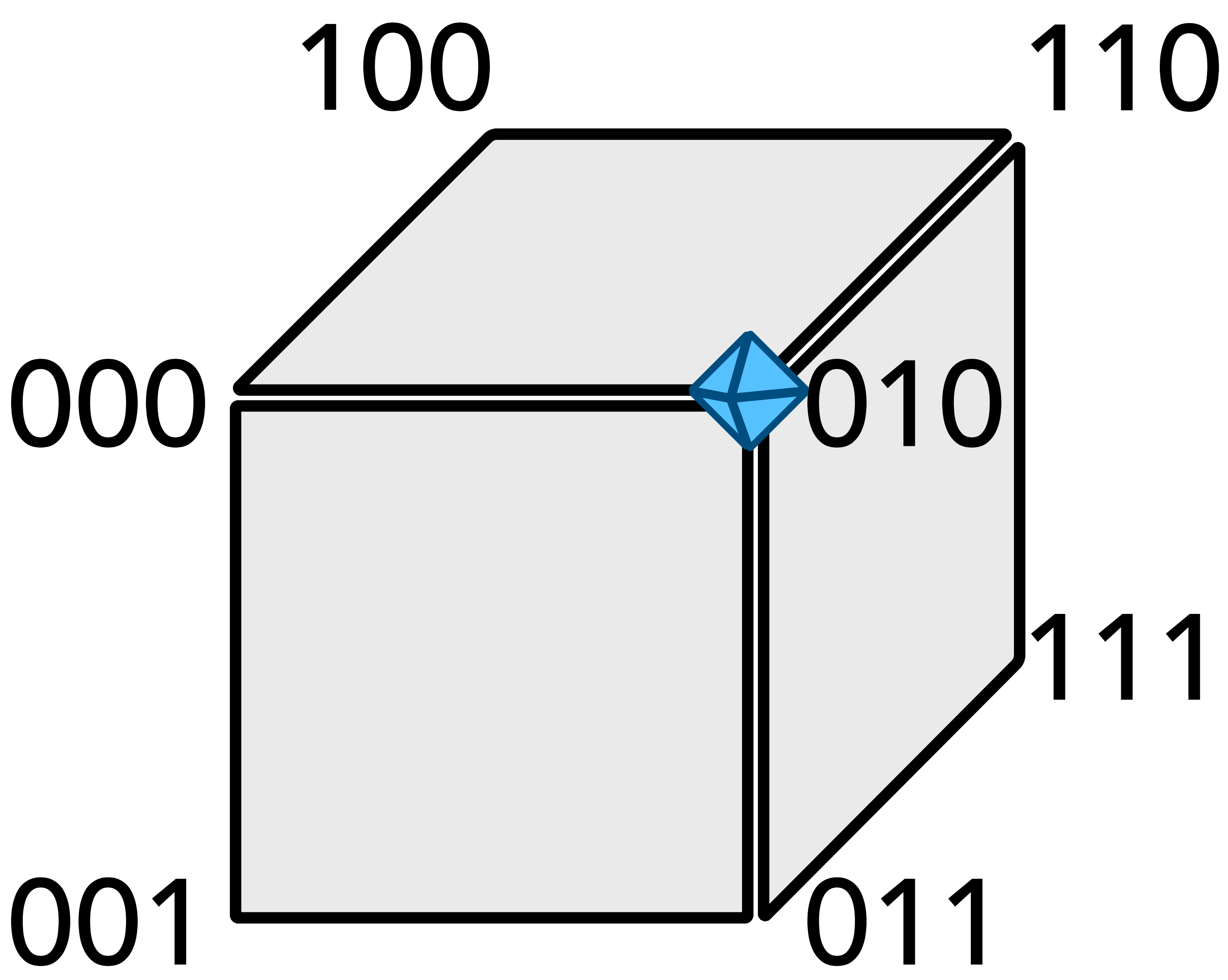

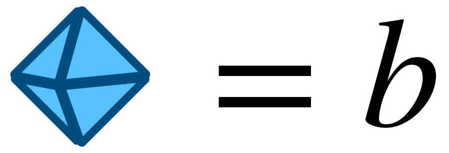

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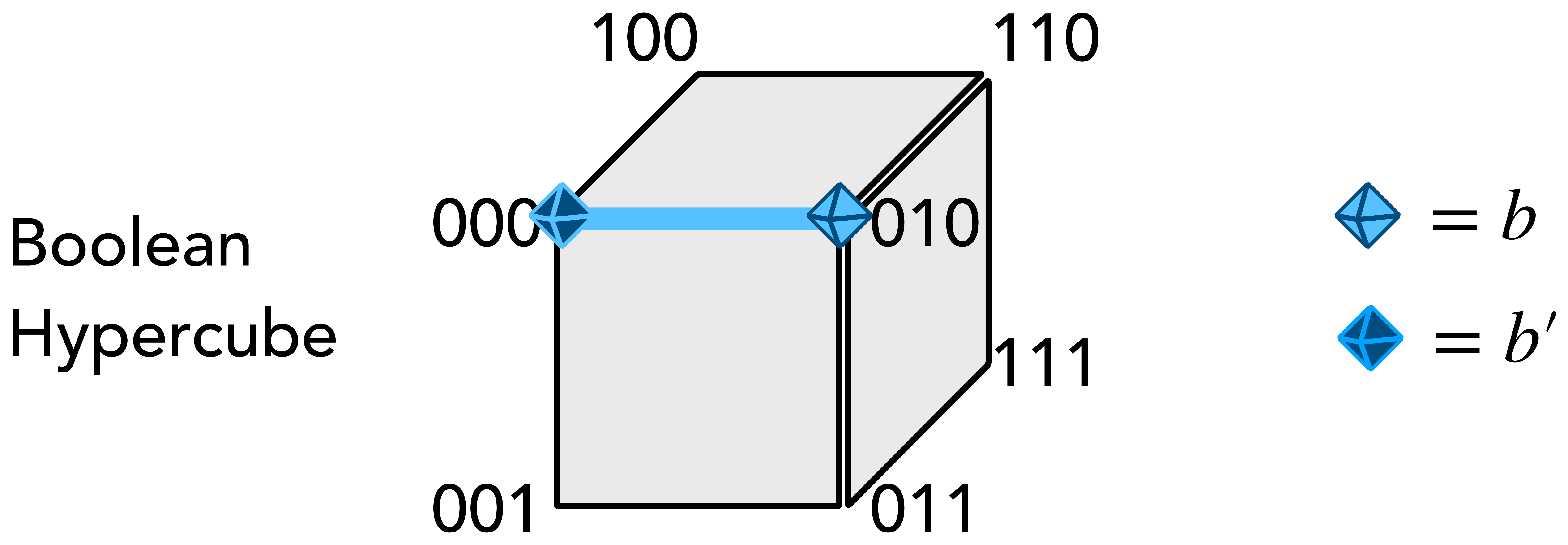
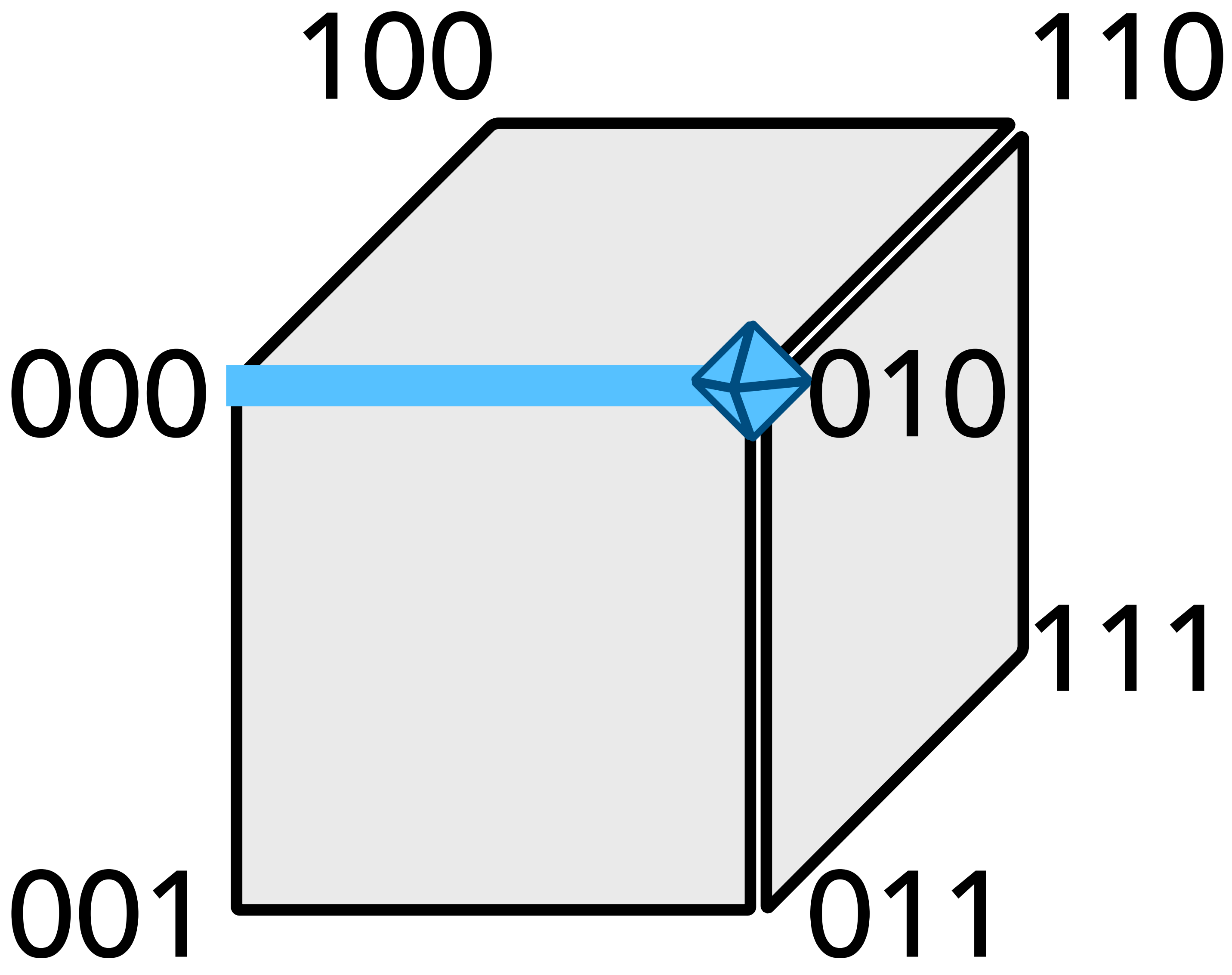


Relaxation Time

- Let $\pi(b) = |\langle b|\psi\rangle|^2$ be the **measurement distribution**.
- Consider a random walk on n-bit Boolean hypercube.

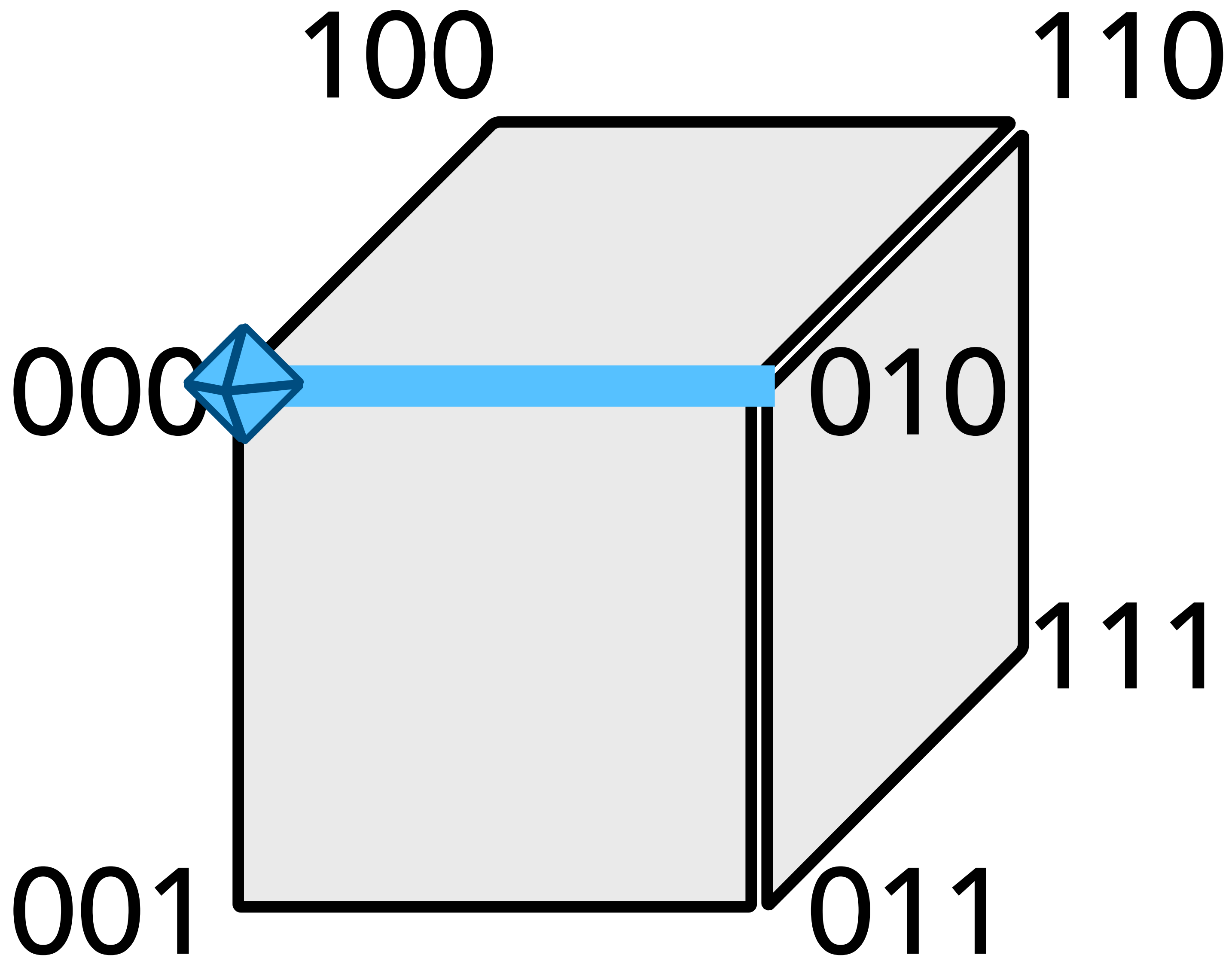
With prob.

$$\frac{\pi(b)}{\pi(b)+\pi(b')}$$



With prob.

$$\frac{\pi(b')}{\pi(b)+\pi(b')}$$

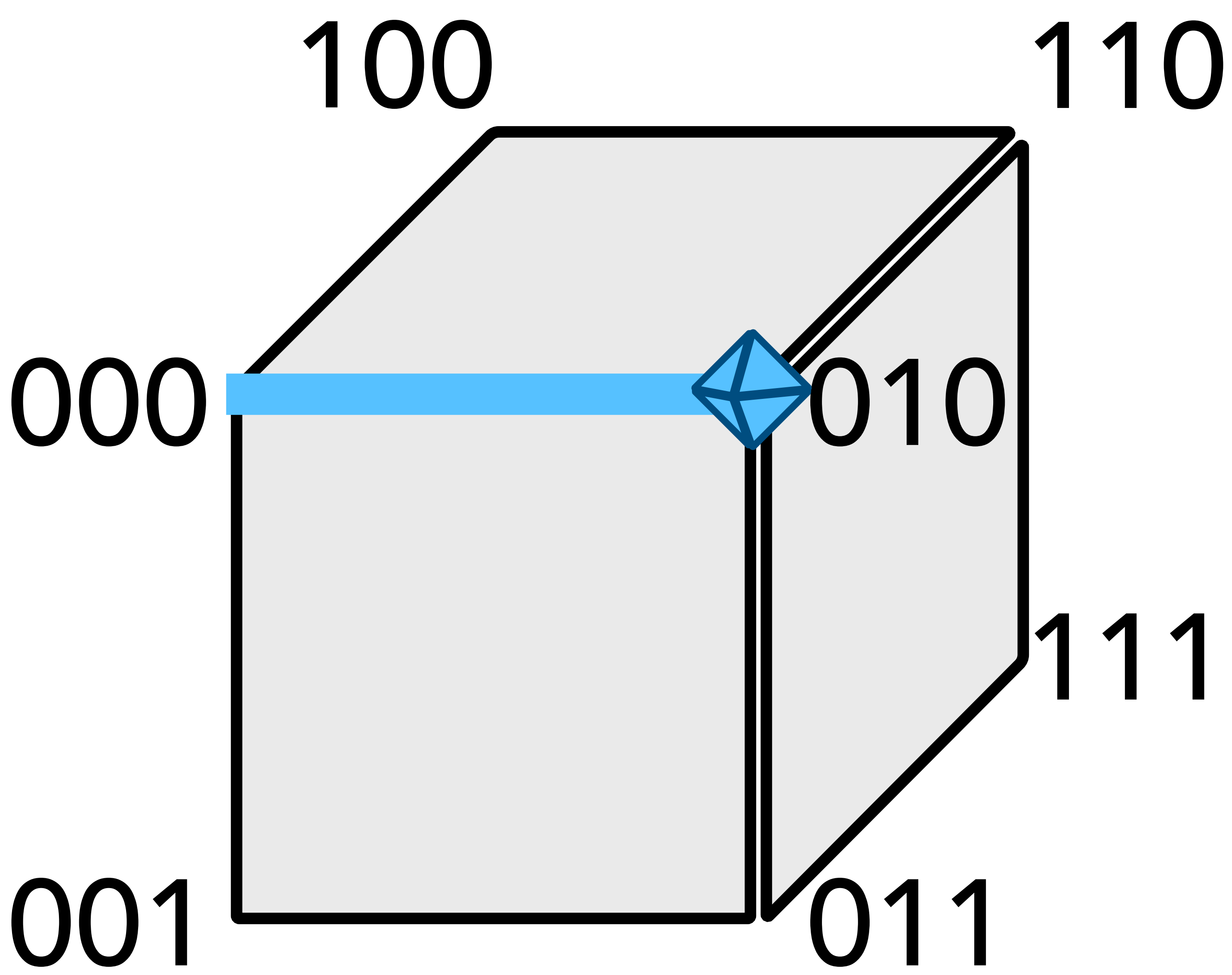


Relaxation Time

- Let $\pi(b) = |\langle b|\psi\rangle|^2$ be the **measurement distribution**.
- τ is the time the random talk takes to relax to stationary π.

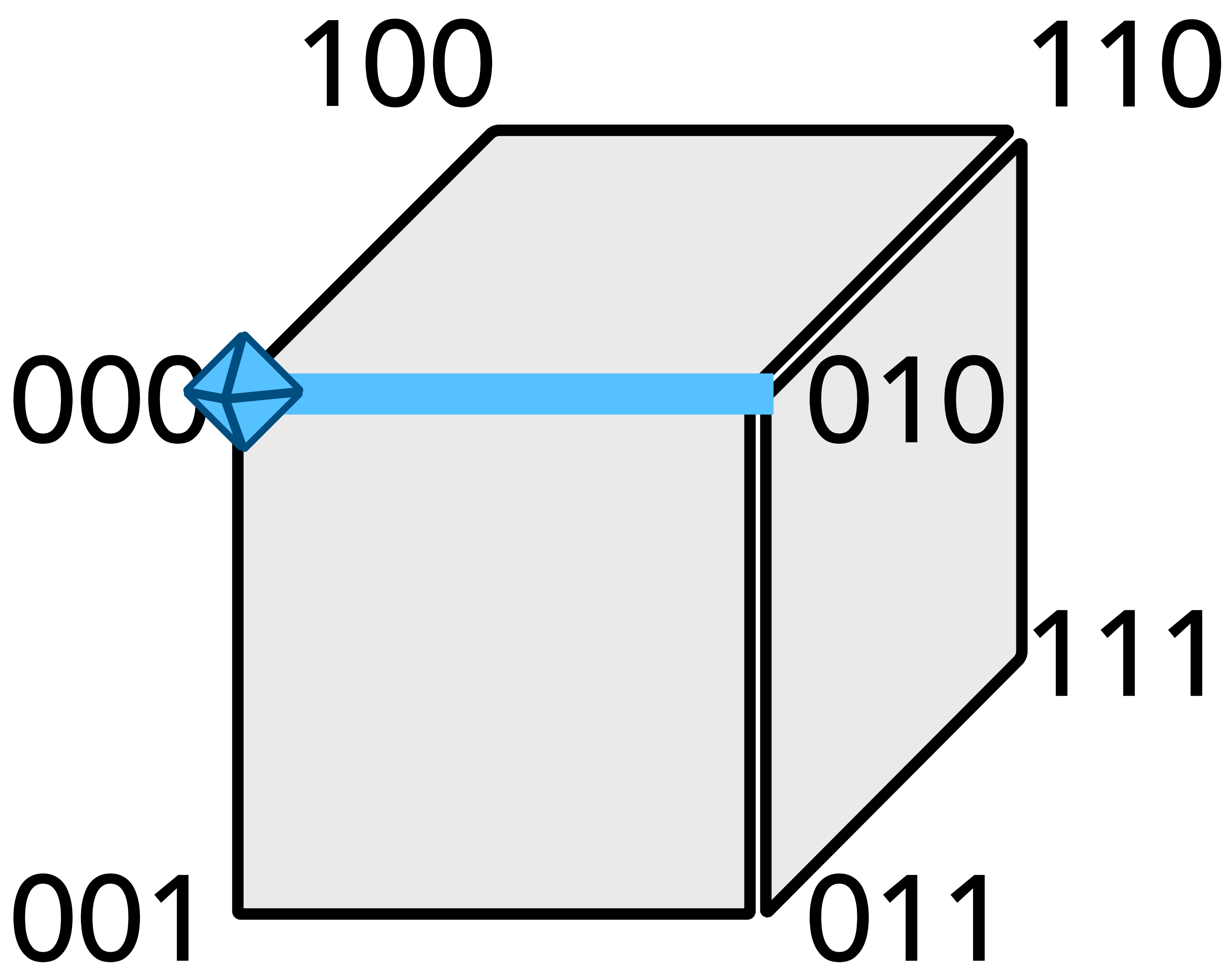
With prob.

$$\frac{\pi(b)}{\pi(b) + \pi(b')}$$



With prob.

$$\frac{\pi(b')}{\pi(b) + \pi(b')}$$



Question: Relation to Fidelity

How does $\mathbb{E}[\omega]$ relate to the fidelity $\langle\psi|\rho|\psi\rangle$?

ω is an estimator for the fidelity with the **ideal** 1-qubit state $|\psi_{b_0,b_1}\rangle$

$$\mathbb{E}[\omega] = \frac{1}{n}\sum_{i=1}^{n}\sum_{b_{\neq i}\in\{0,1\}^{n-1}} \mathrm{Tr}\left(\langle b_{\neq i}|\rho|b_{\neq i}\rangle \frac{\langle b_{\neq i}|\psi\rangle\langle\psi|b_{\neq i}\rangle}{\mathrm{Tr}\langle b_{\neq i}|\psi\rangle\langle\psi|b_{\neq i}\rangle}\right)$$

$$= \mathrm{Tr}\left(L_{|\psi\rangle}\cdot\rho\right) \in [0,1]$$

$|\psi\rangle$ — 1

— $1-(1/\tau)$

⋮

—

Spectrum of $L_{|\psi\rangle}$

Question: Relation to Fidelity

$\mathbb{E}[\omega] \geq 1 - \epsilon$ **implies** $\langle \psi | \rho | \psi \rangle \geq 1 - \tau\epsilon$

$\langle \psi | \rho | \psi \rangle \geq 1 - \epsilon$ **implies** $\mathbb{E}[\omega] \geq 1 - \epsilon$

$$\mathbb{E}[\omega] = \frac{1}{n} \sum_{i=1}^{n} \sum_{b_{\neq i} \in \{0,1\}^{n-1}} \mathrm{Tr}\left(\langle b_{\neq i} | \rho | b_{\neq i} \rangle \frac{\langle b_{\neq i} | \psi \rangle\langle \psi | b_{\neq i} \rangle}{\mathrm{Tr}\langle b_{\neq i} | \psi \rangle\langle \psi | b_{\neq i} \rangle} \right)$$

$$= \mathrm{Tr}\left(L_{|\psi\rangle} \cdot \rho \right) \in [0,1]$$

$|\psi\rangle$ — 1

— $1 - (1/\tau)$

⋮

—

Spectrum of $L_{|\psi\rangle}$

Certification

Theorem 1

For an n-qubit state $|\psi\rangle$ with relax. time τ, we can certify that ρ is close to $|\psi\rangle\langle\psi|$ with $\mathcal{O}(\tau)$ single-qubit measurements.

- The certification procedure applies to any ρ.

Certification

Theorem 2

For almost all n-qubit state $|\psi\rangle$, we can certify that ρ is close to $|\psi\rangle\langle\psi|$ using only $\mathcal{O}(n^2)$ single-qubit measurements.

- The certification procedure applies to any ρ.
- $\mathcal{O}(n^2)$ is enough even when $|\psi\rangle$ has $\exp(n)$ circuit complexity.

Question: Applications

What can we use state certification for?

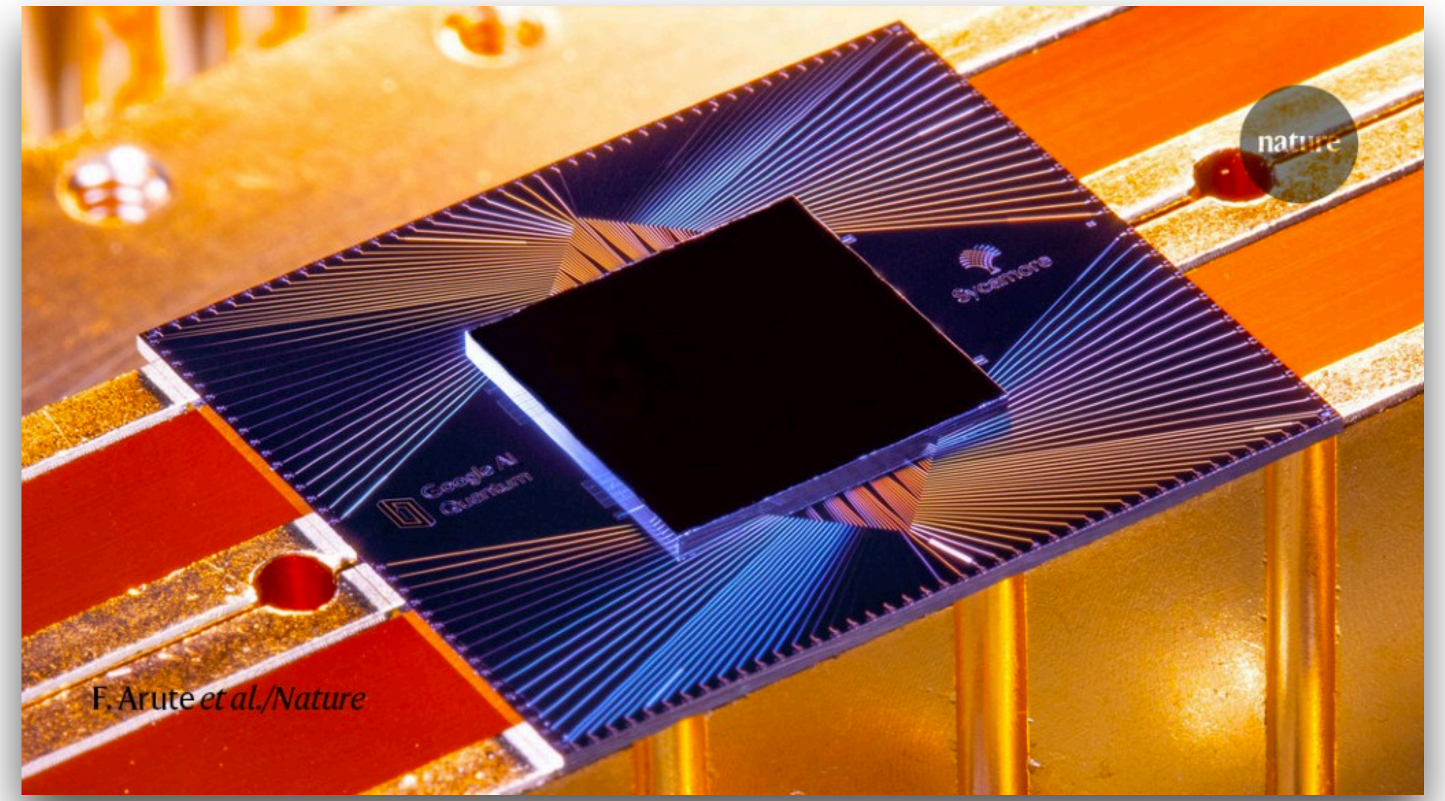
Question: Applications

What can we use state certification for?

Example 1

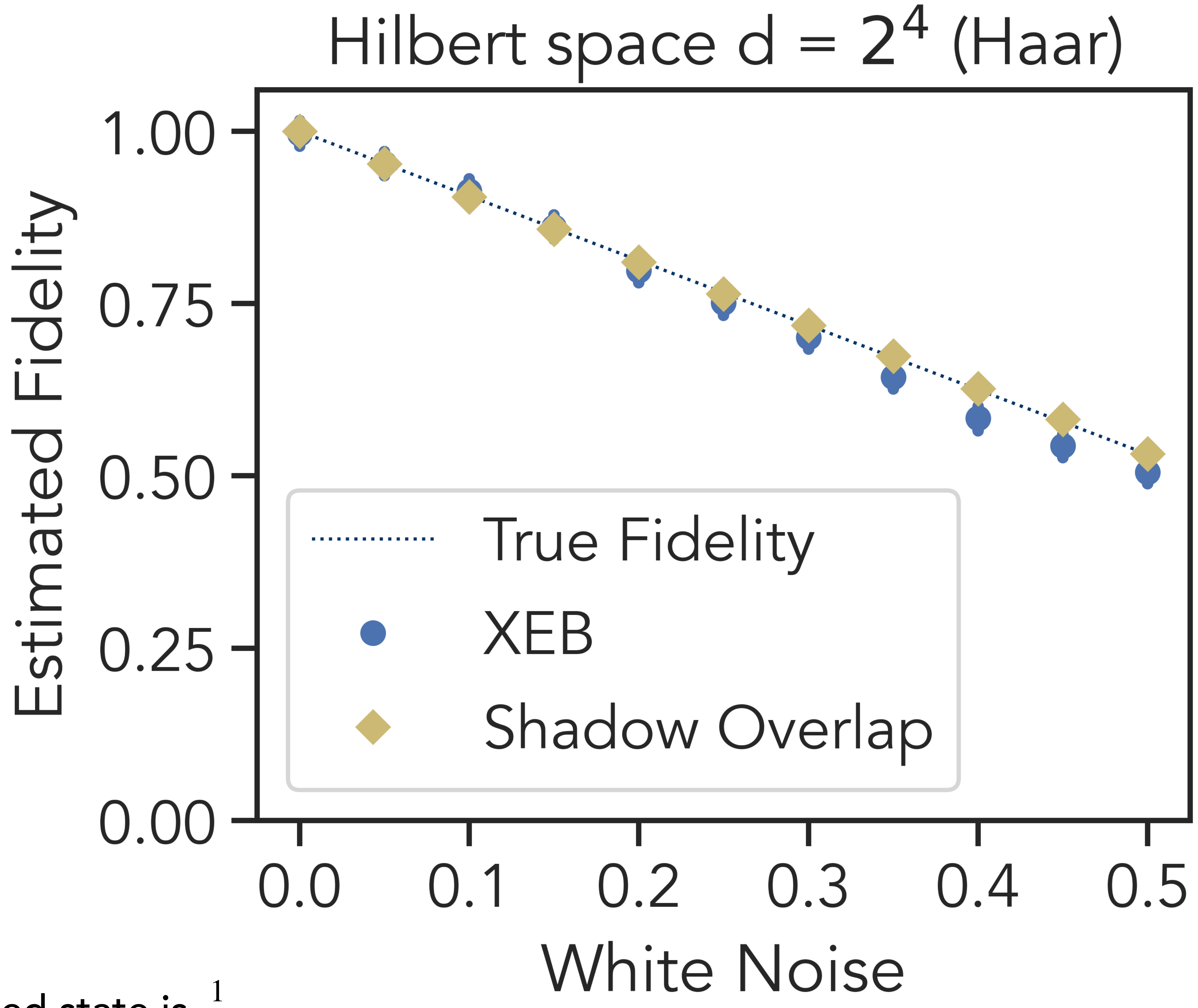
Benchmarking

Certification enables us to test our quantum devices



Benchmarking quantum devices

4-qubit Haar random state
White Noise

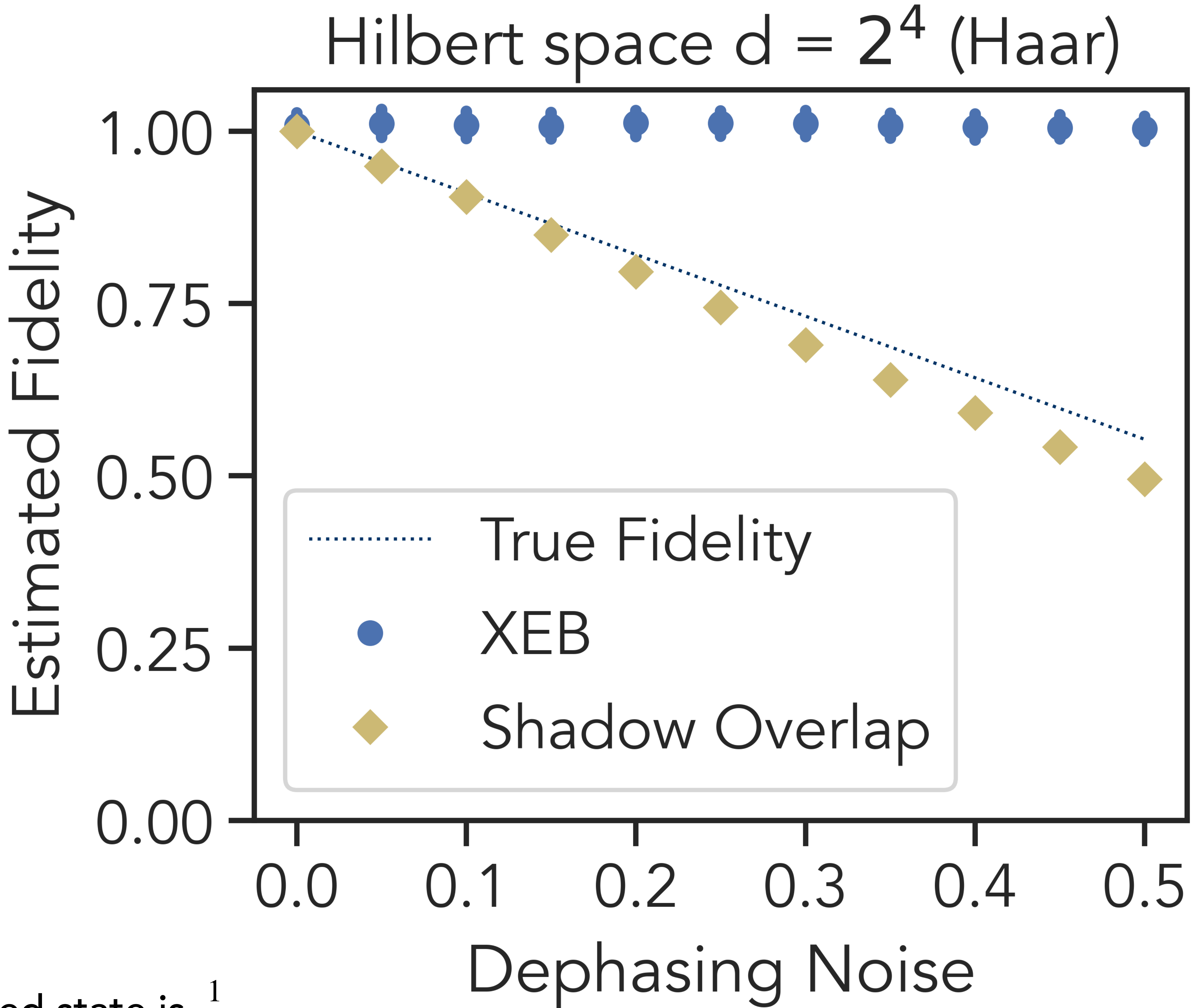


*Shadow overlap normalized s.t., target state is 1, maximally mixed state is $\frac{1}{2^n}$

Benchmarking quantum devices

4-qubit Haar random state

Dephasing Noise



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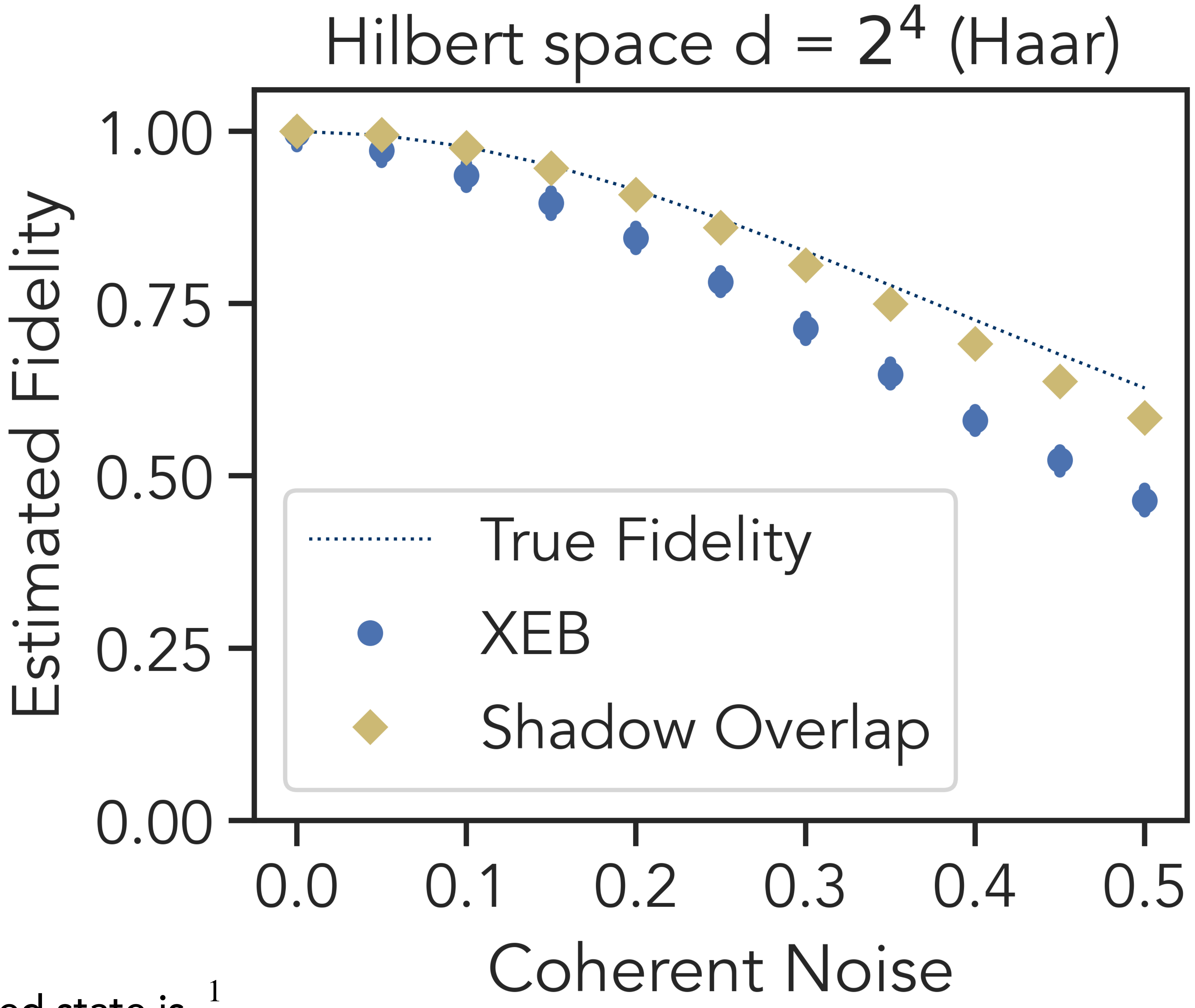
Benchmarking quantum devices

4-qubit Haar random state

Coherent Noise



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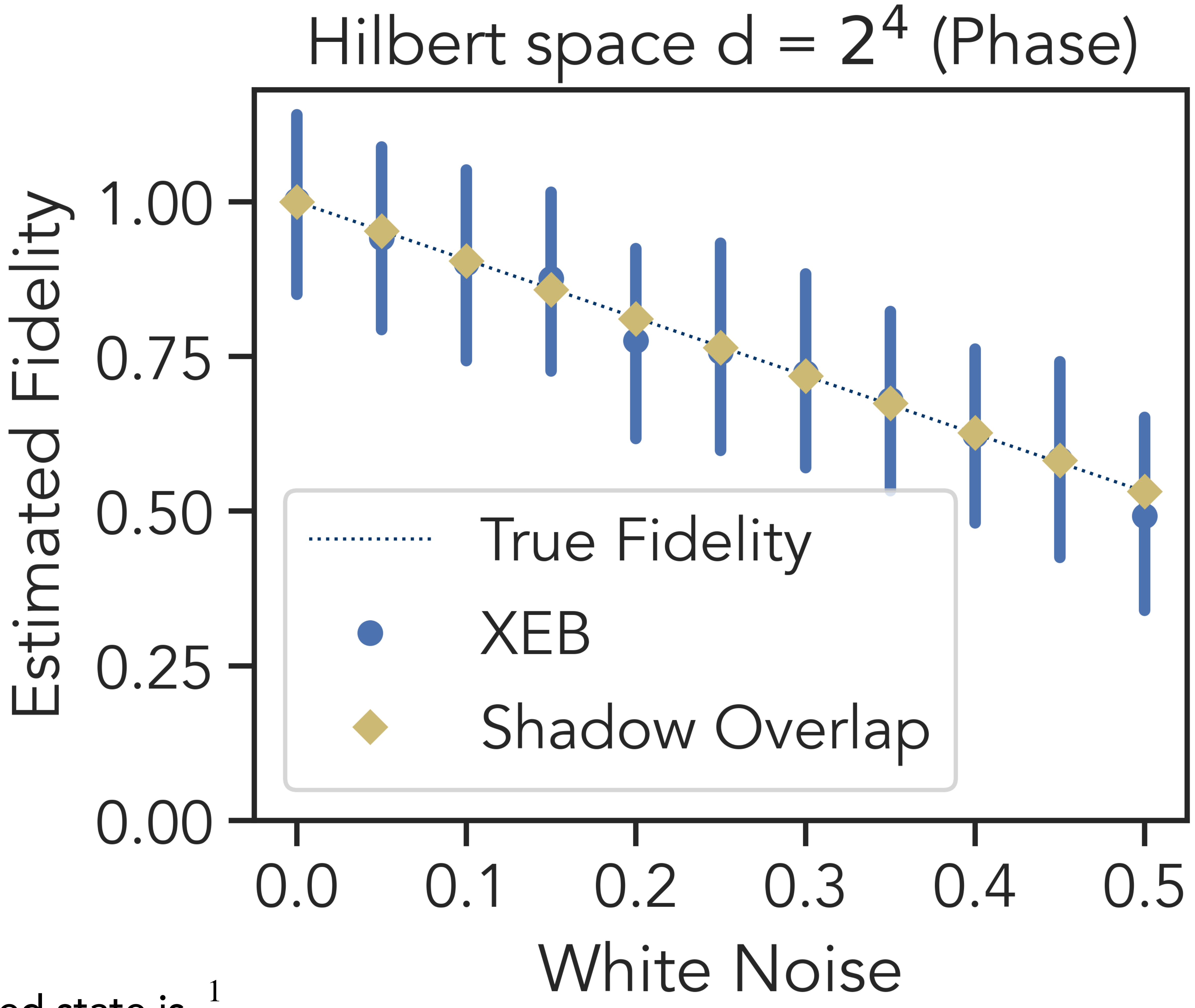
Benchmarking quantum devices

4-qubit random structured state

White Noise

$$|\psi\rangle = U_{\text{phase}} \bigotimes_{i=1}^{4} |\psi_i\rangle$$



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Benchmarking quantum devices

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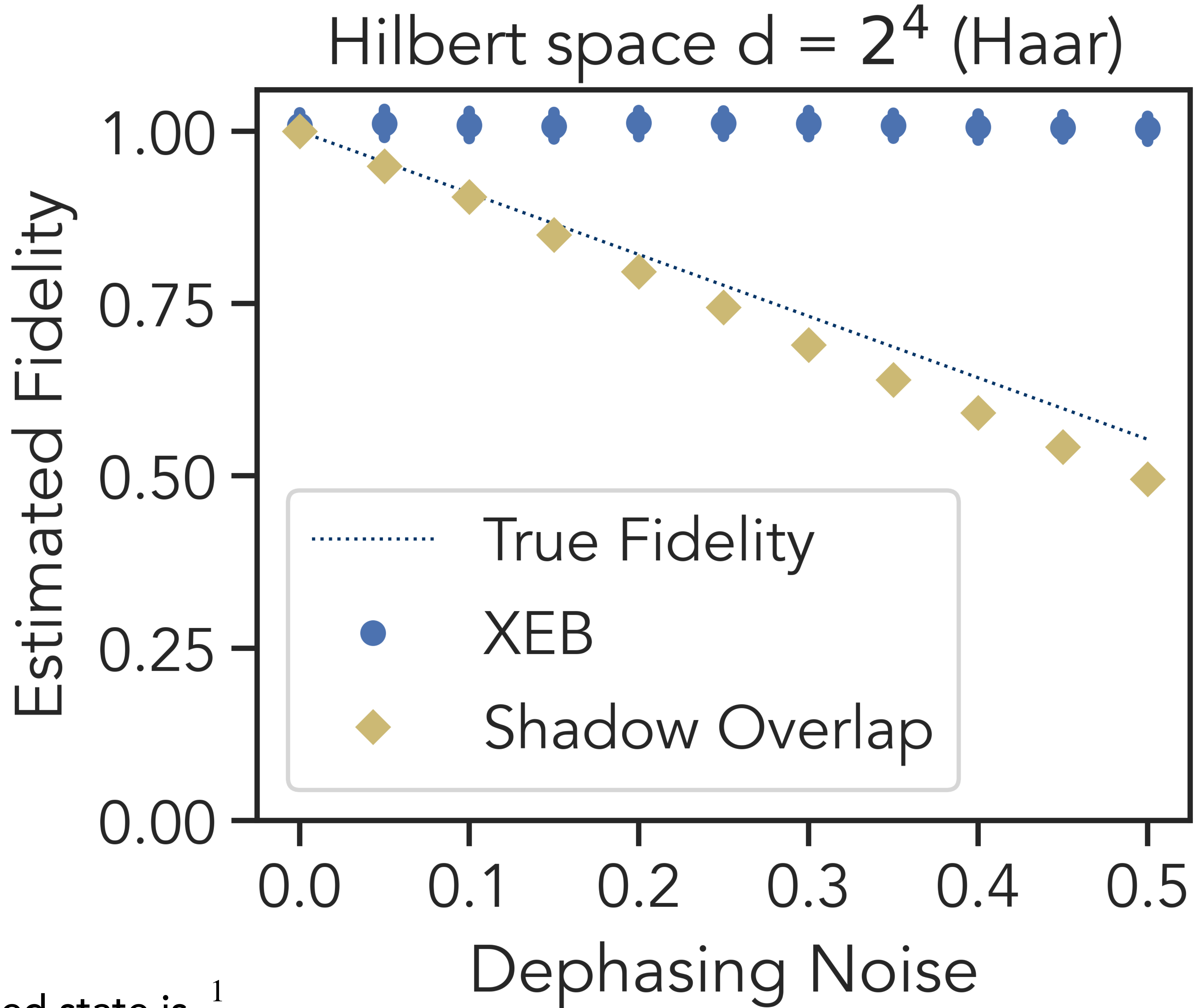

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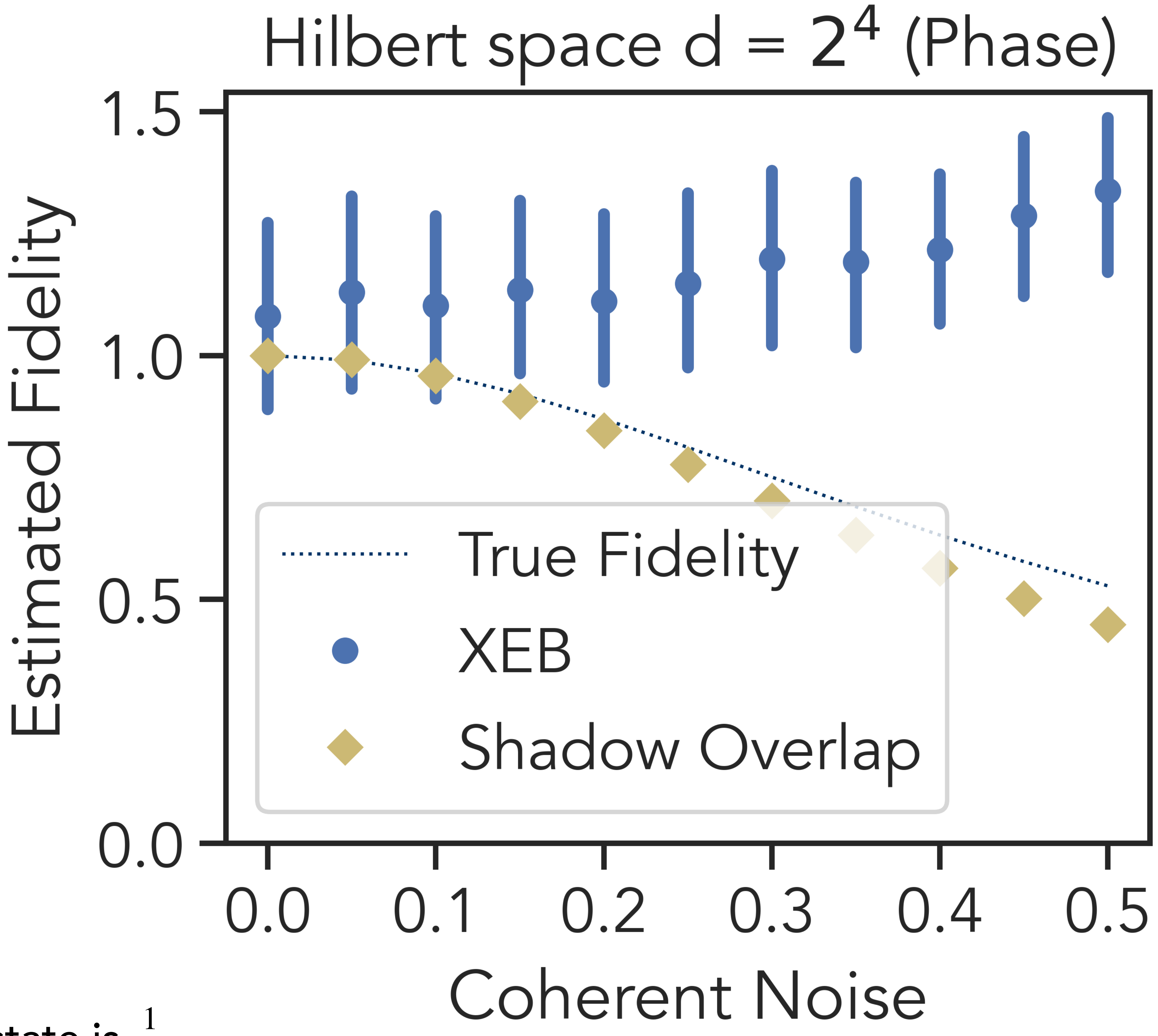
Benchmarking quantum devices

4-qubit random structured state

Coherent Noise

$$|\psi\rangle = U_{\text{phase}} \bigotimes_{i=1}^{4} |\psi_i\rangle$$



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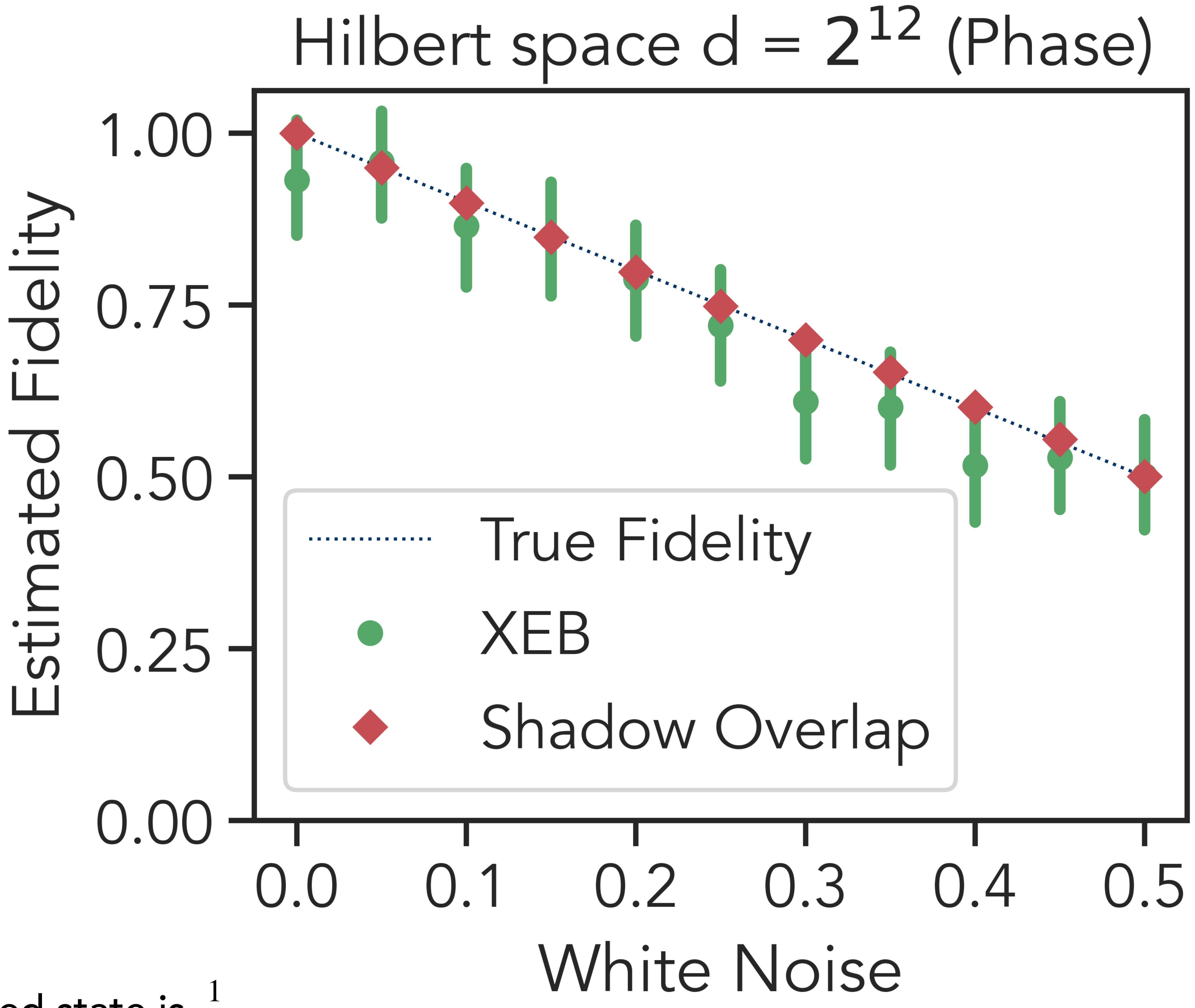
Benchmarking quantum devices

12-qubit random structured state

White Noise

$$|\psi\rangle = U_{\text{phase}} \bigotimes_{i=1}^{4} |\psi_i\rangle$$



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Benchmarking quantum devices

12-qubit random structured state

Dephasing Noise

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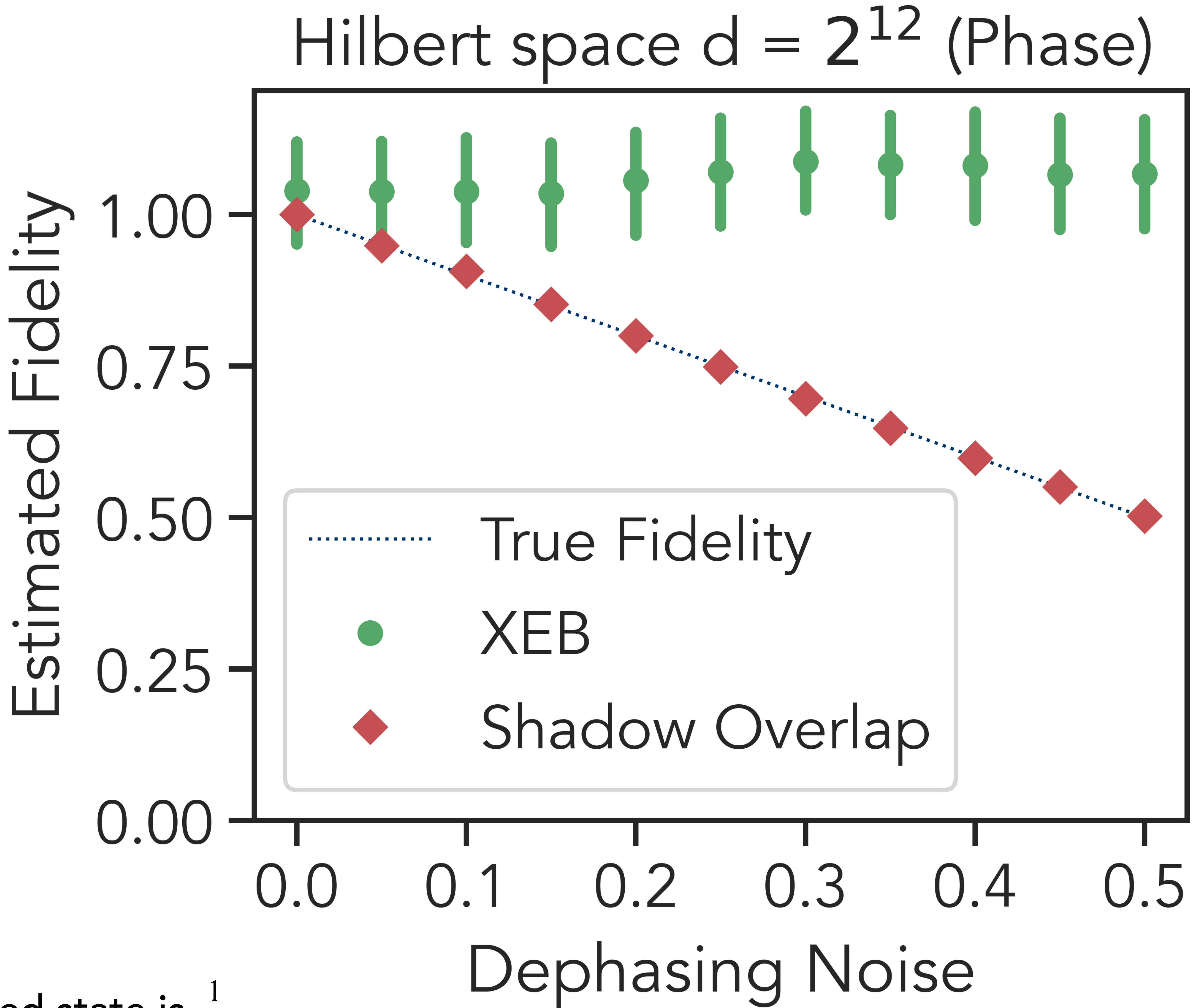

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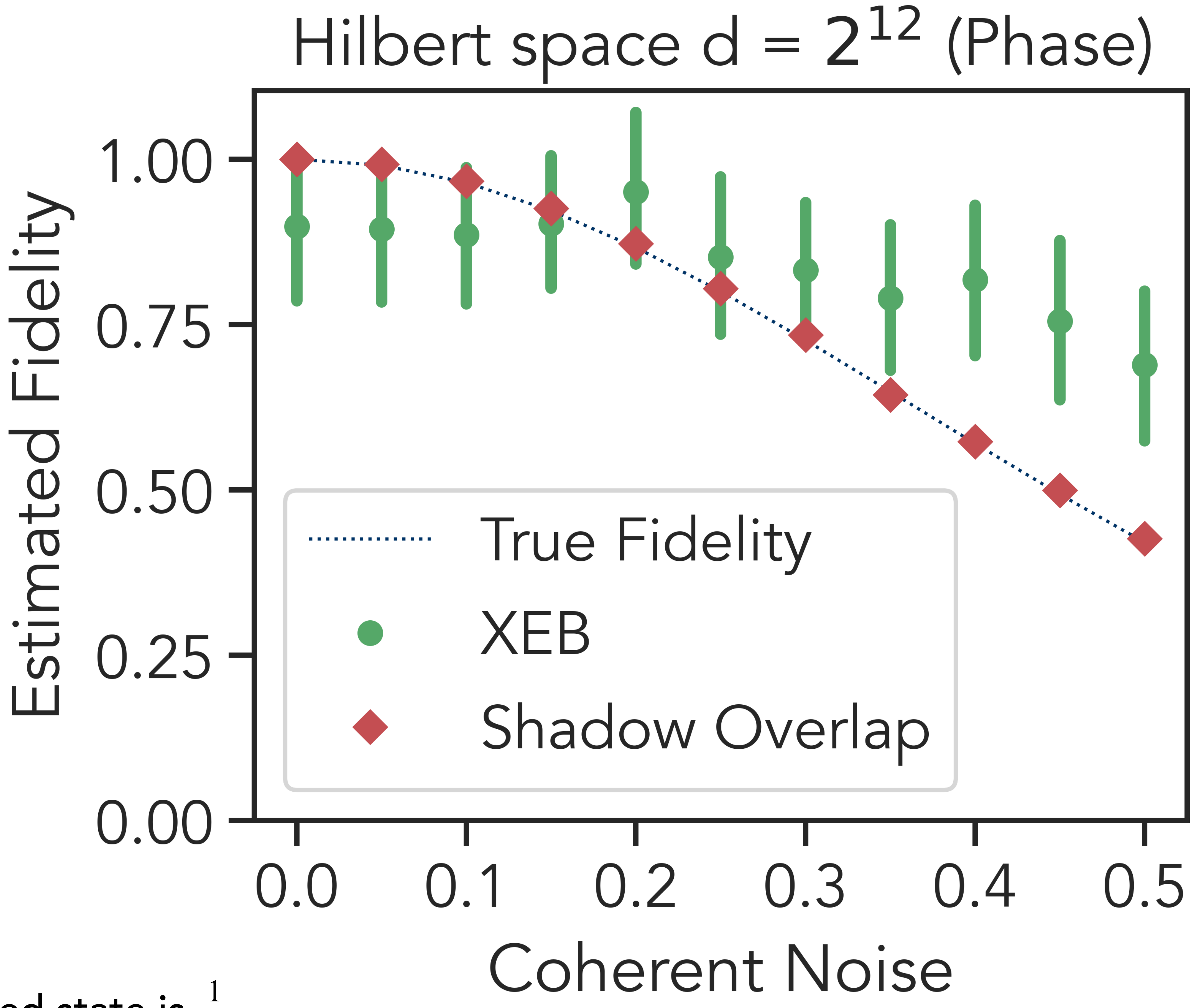
Benchmarking quantum devices

12-qubit random structured state
Coherent Noise

$$|\psi\rangle = U_{\text{phase}} \bigotimes_{i=1}^{4} |\psi_i\rangle$$



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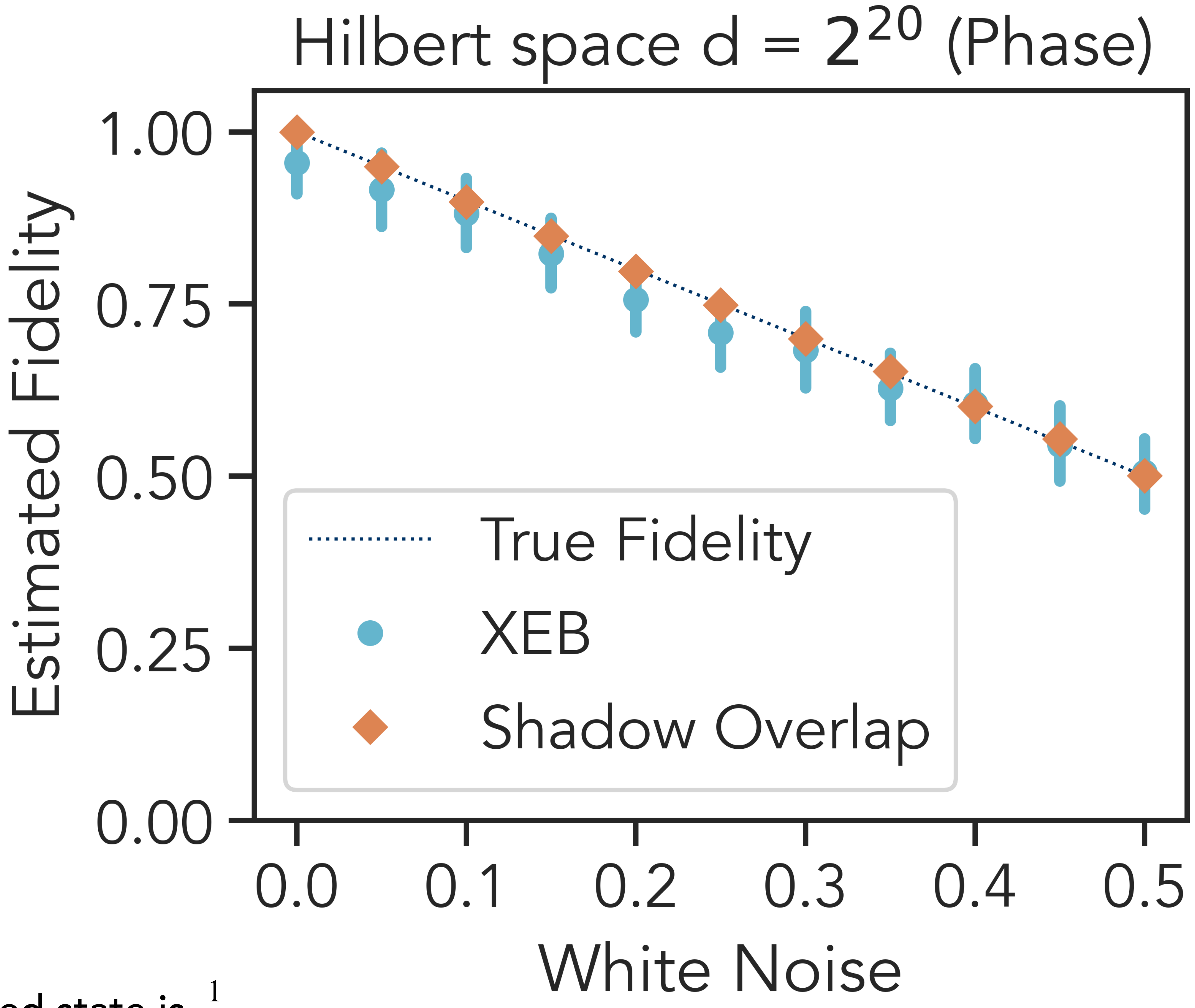
Benchmarking quantum devices

20-qubit random structured state

White Noise

$$|\psi\rangle = U_{\text{phase}} \bigotimes_{i=1}^{4} |\psi_i\rangle$$



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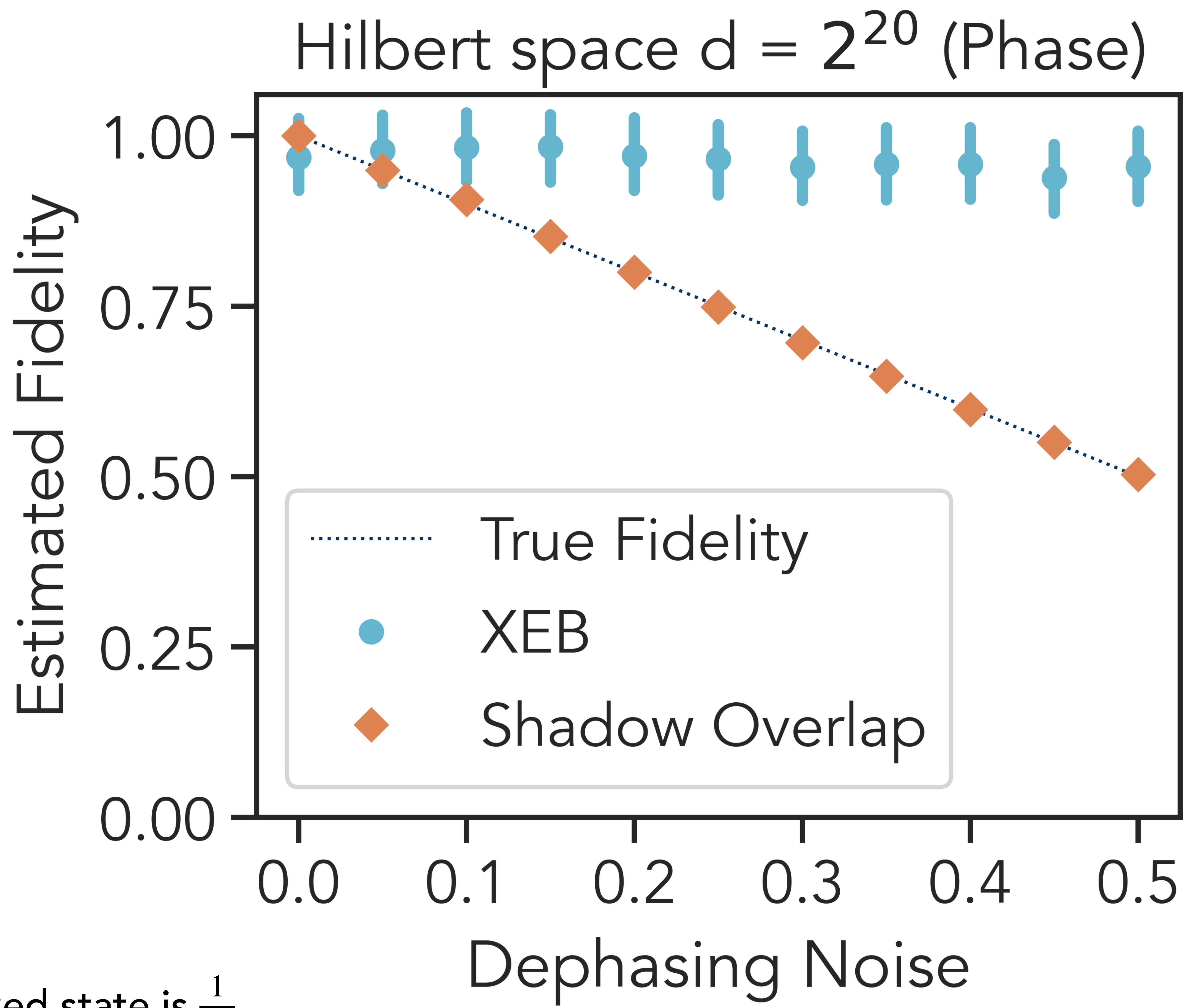
Benchmarking quantum devices

20-qubit random structured state

Dephasing Noise

$$|\psi\rangle = U_{\text{phase}} \bigotimes_{i=1}^{4} |\psi_i\rangle$$



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Benchmarking quantum devices

20-qubit random structured state

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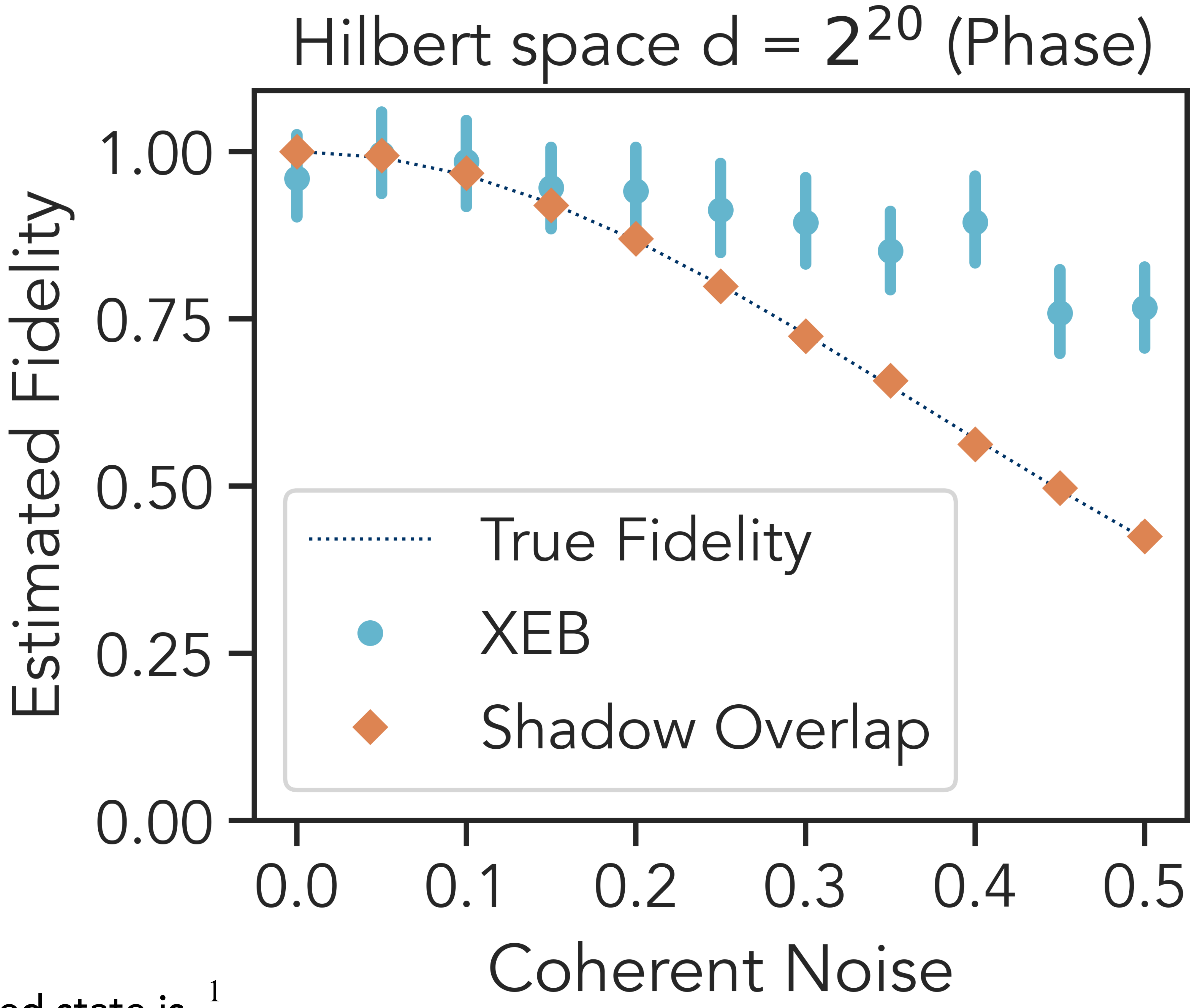


*Shadow overlap normalized s.t., target state is 1, maximally mixed state is $\frac{1}{2^n}$

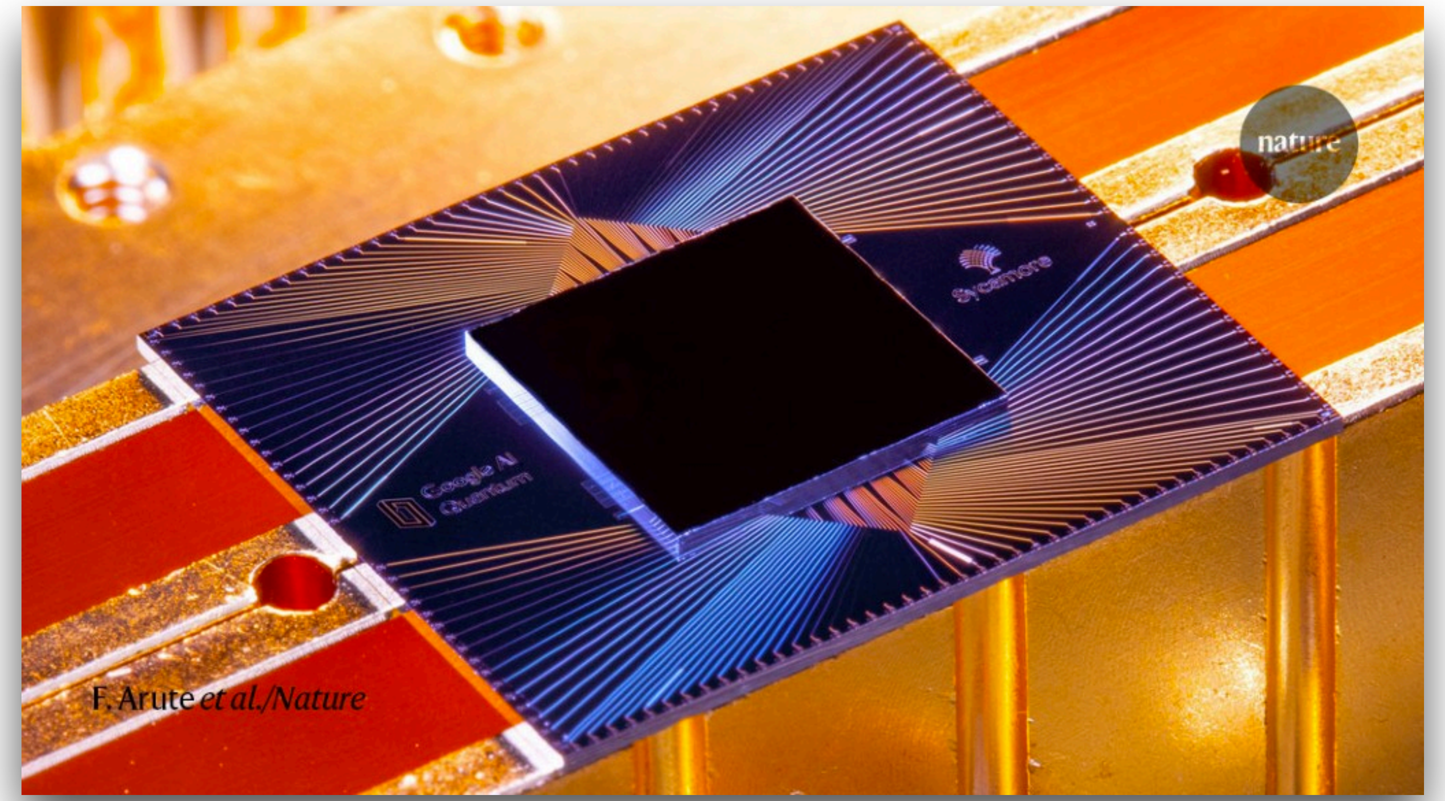
Question: Applications

What can we use state certification for?

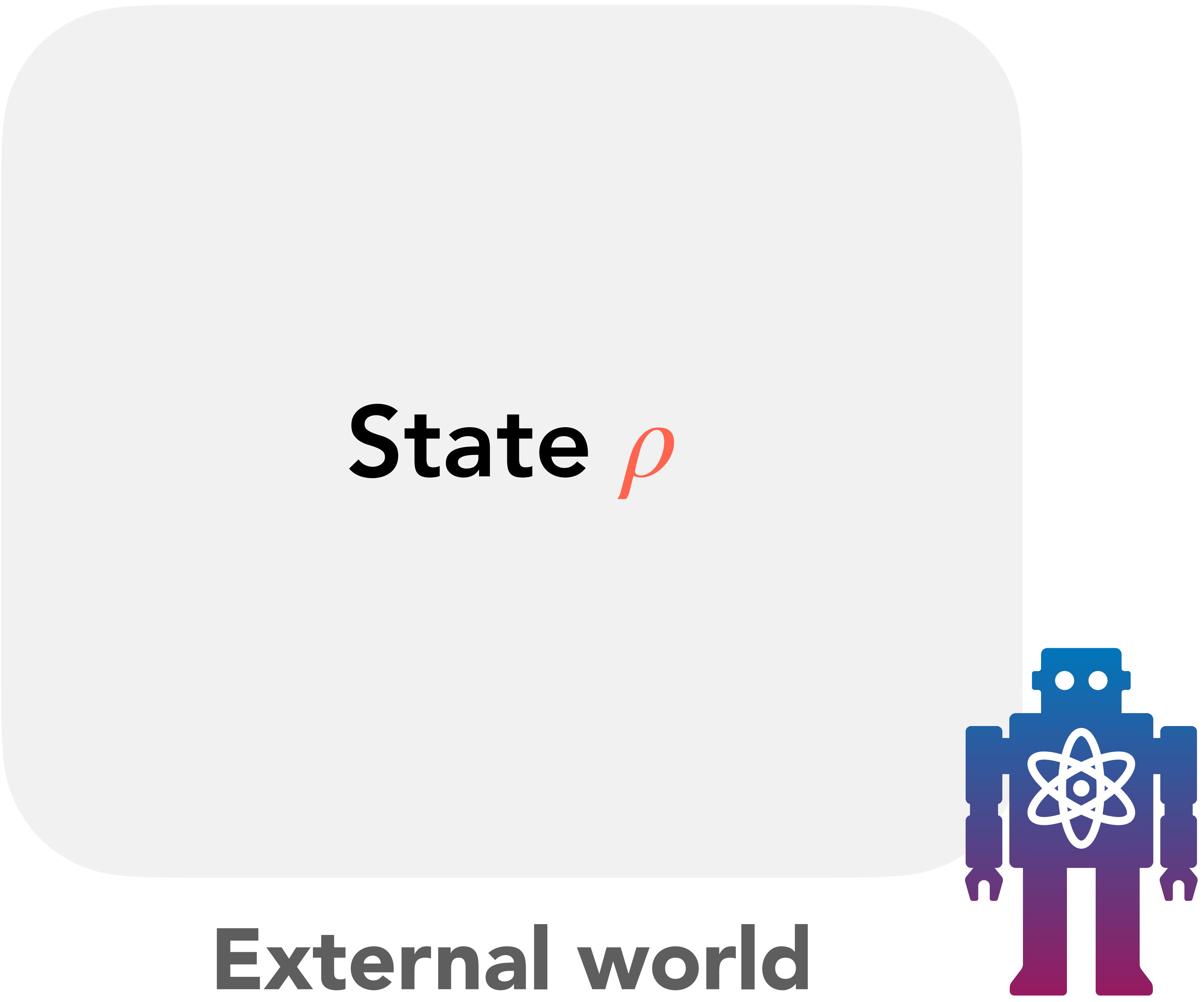
Example 1

Benchmarking

Certification enables us to test our quantum devices



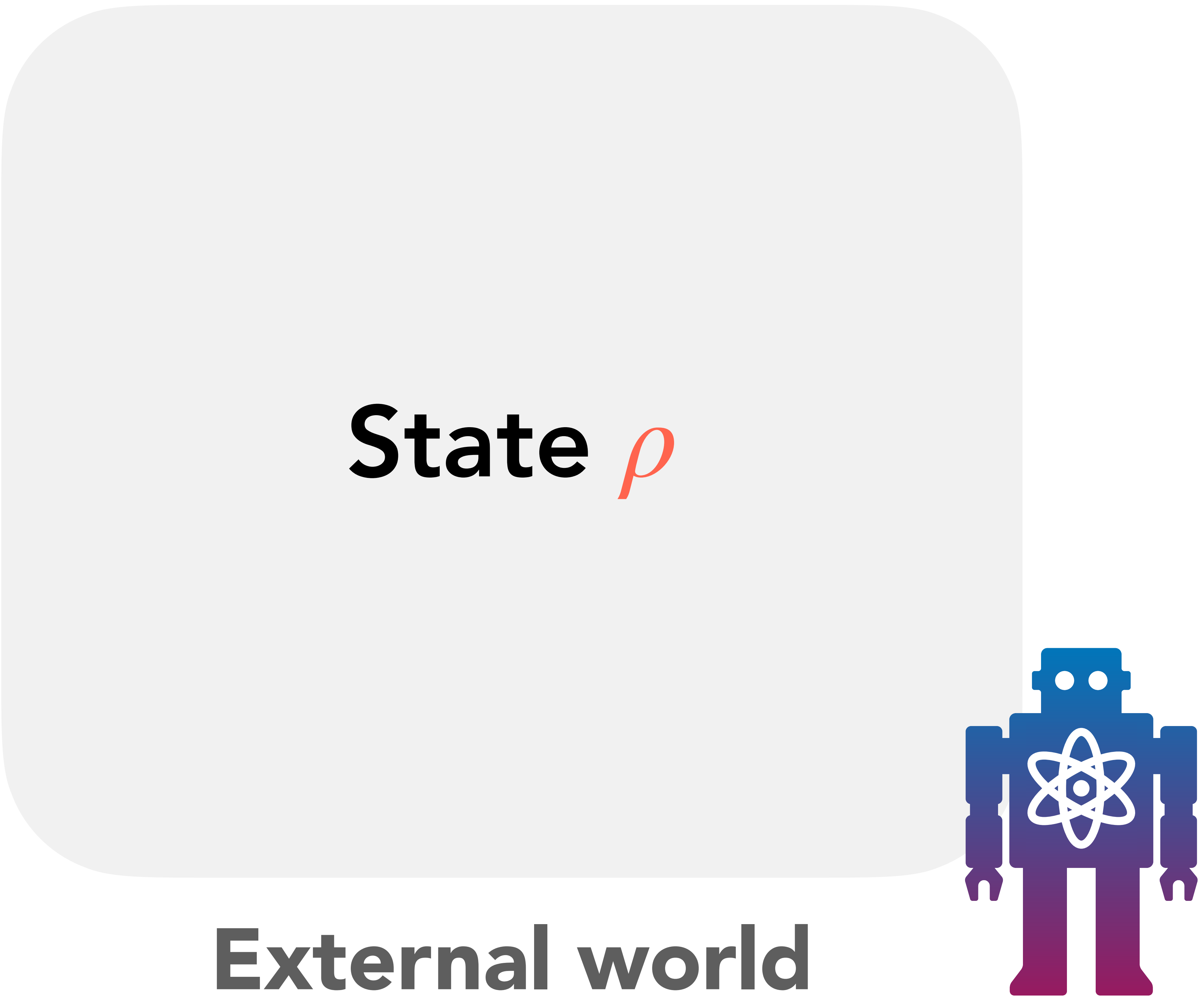
Question: Certify $\mapsto$ Learn



Given a parameterized family of states $|\psi(\vec{x})\rangle$,

how can we learn the $|\psi(\vec{x}_\star)\rangle$ closest to ρ from few single-qubit measurements?

Question: Neural quantum states



Given a trained **neural network** representation of $|\psi\rangle$, i.e., NN: $x \in \{0,1\}^n \mapsto \langle x | \psi \rangle \in \mathbb{C}$.

How to efficiently certify that the **neural network** is correct?

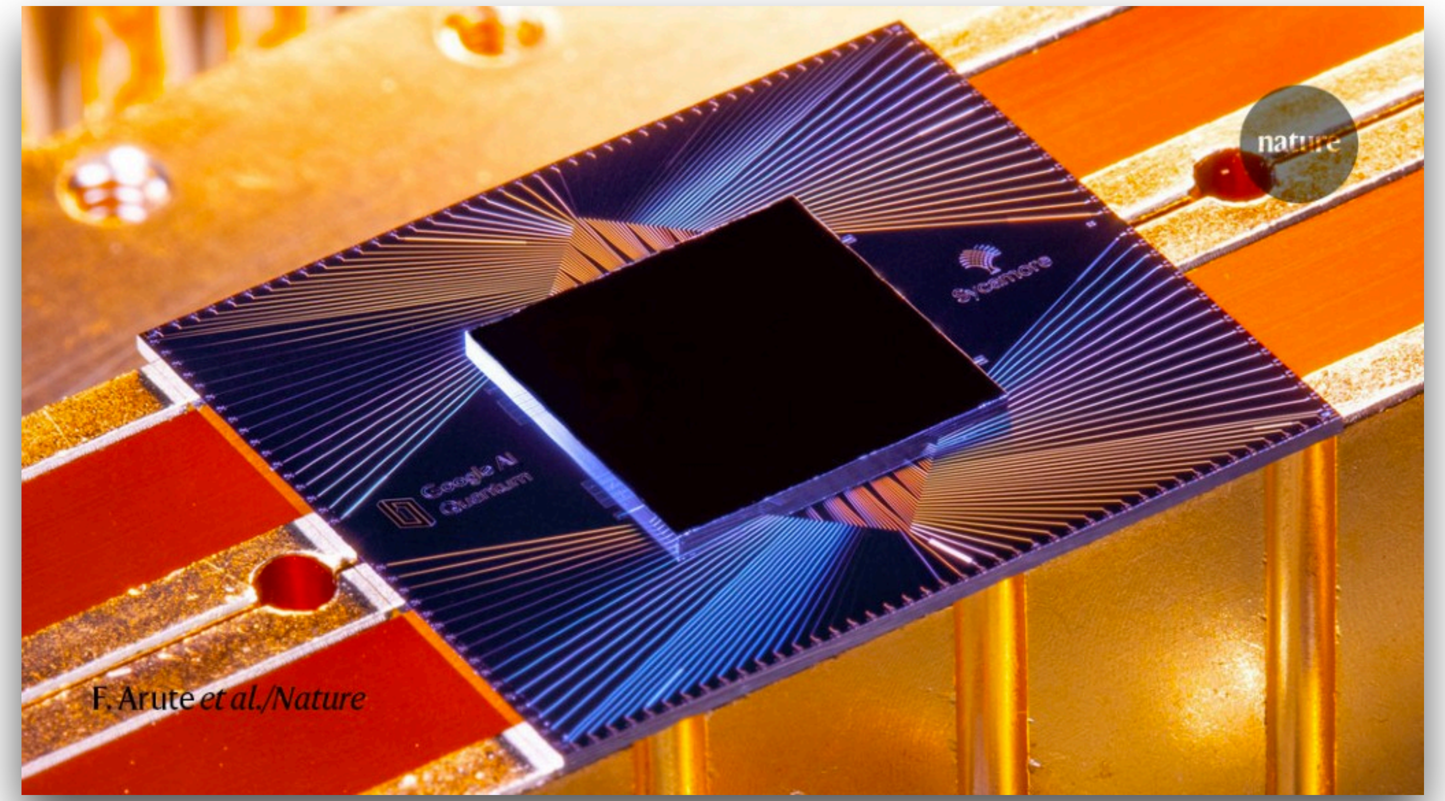
Question: Applications

What can we use state certification for?

Example 1

Benchmarking

Certification enables us to test our quantum devices



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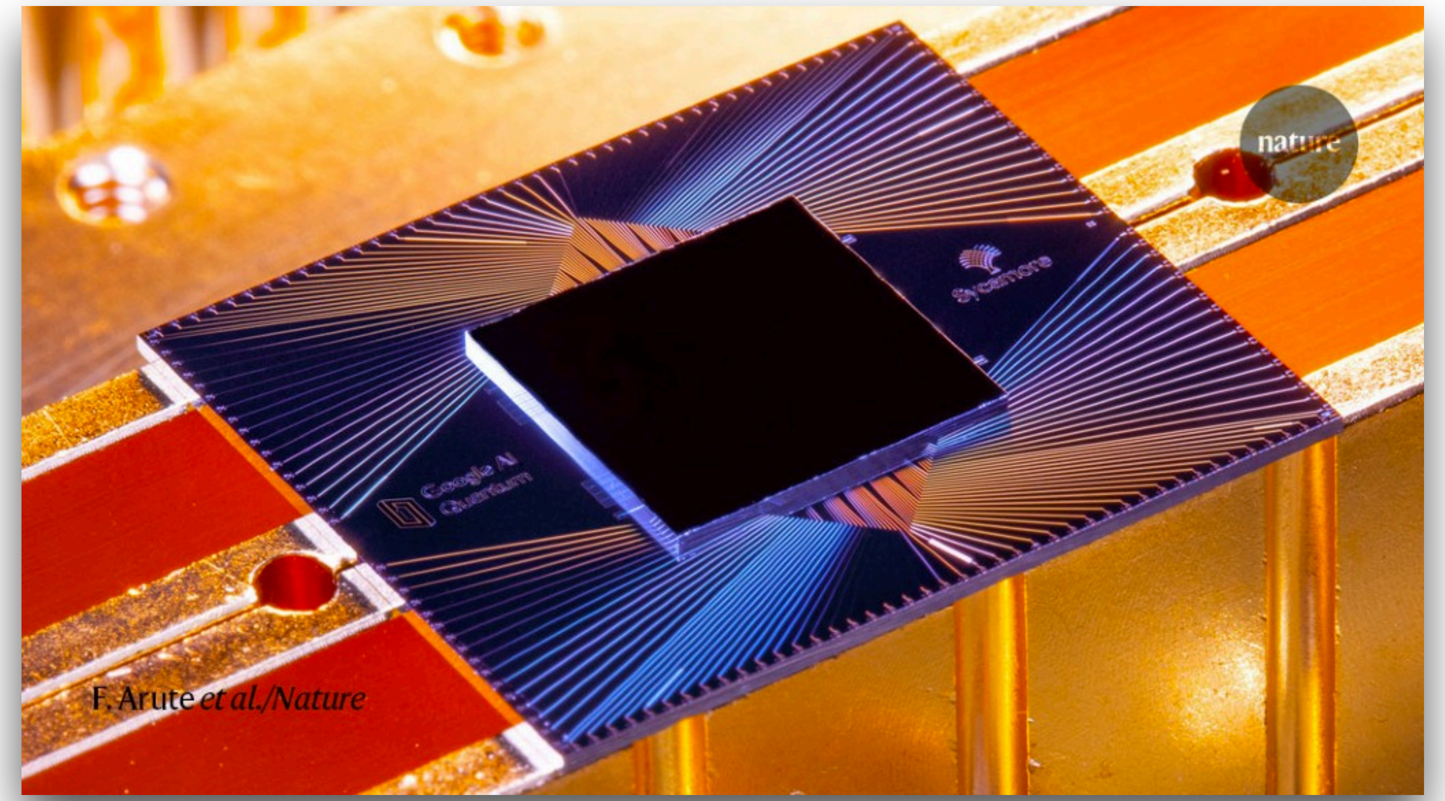
Benchmarking

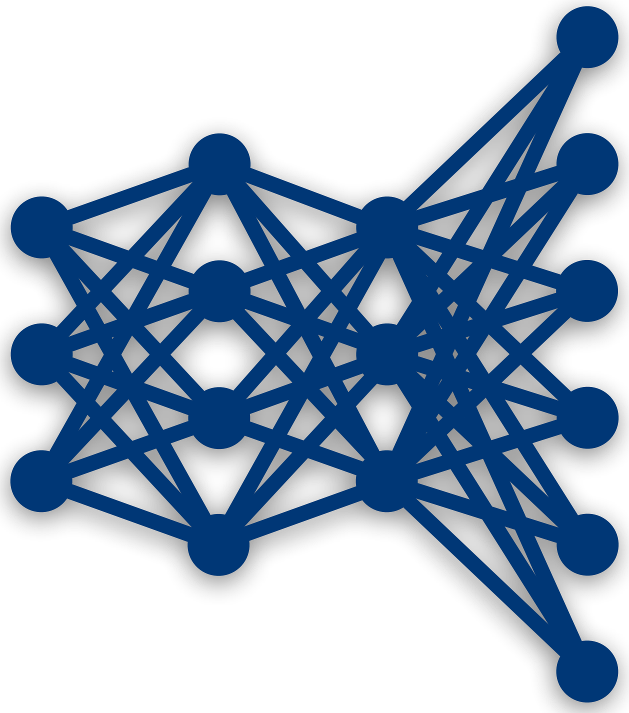
Certification enables us to test our quantum devices



Example 2

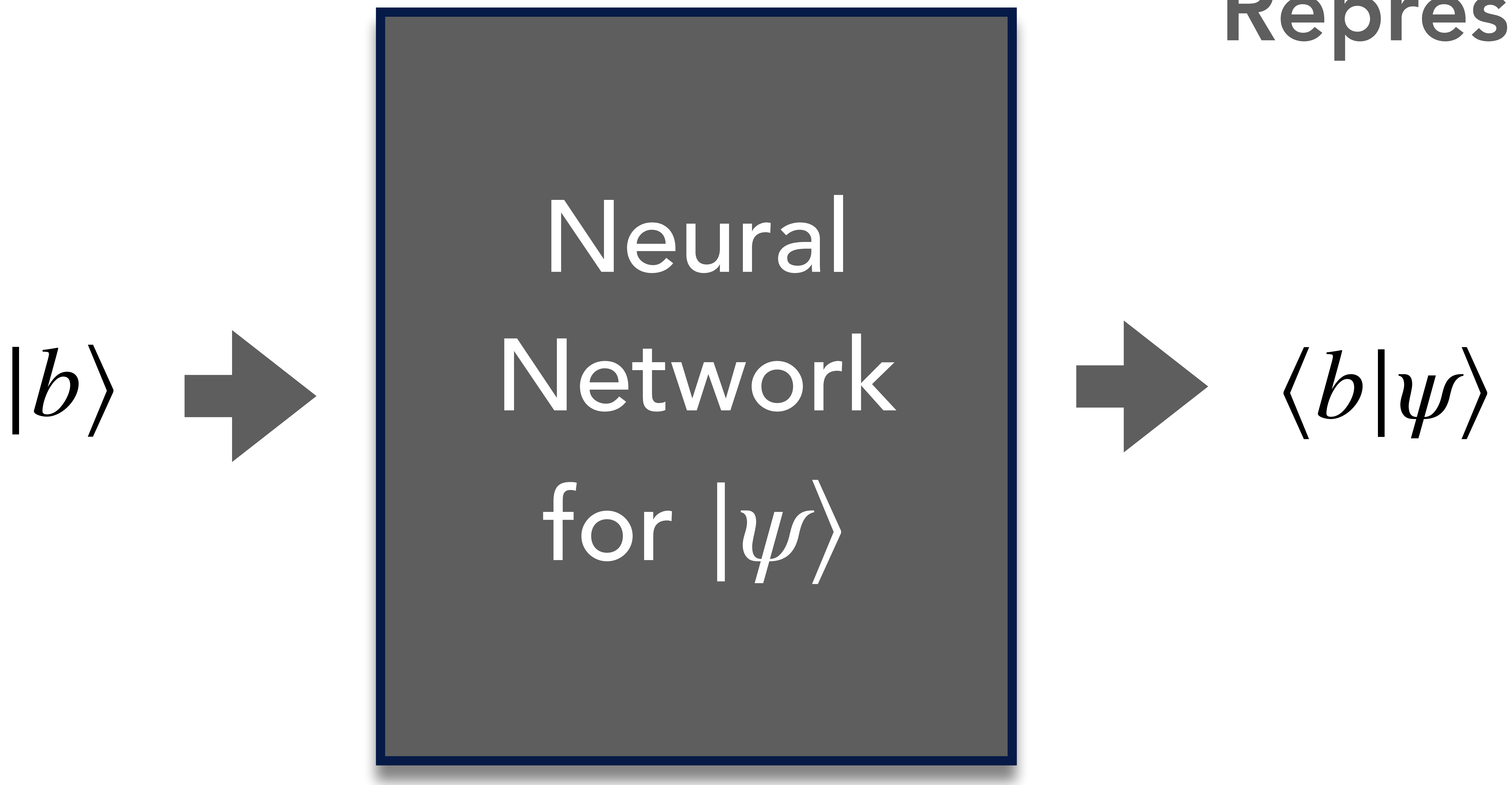
Certify ML models

State certification can be used to train/certify ML models, such as neural quantum states.



Training/Certifying Neural Q States

Represent $|\psi\rangle$



Standard Neural Quantum State

Training/Certifying Neural Q States

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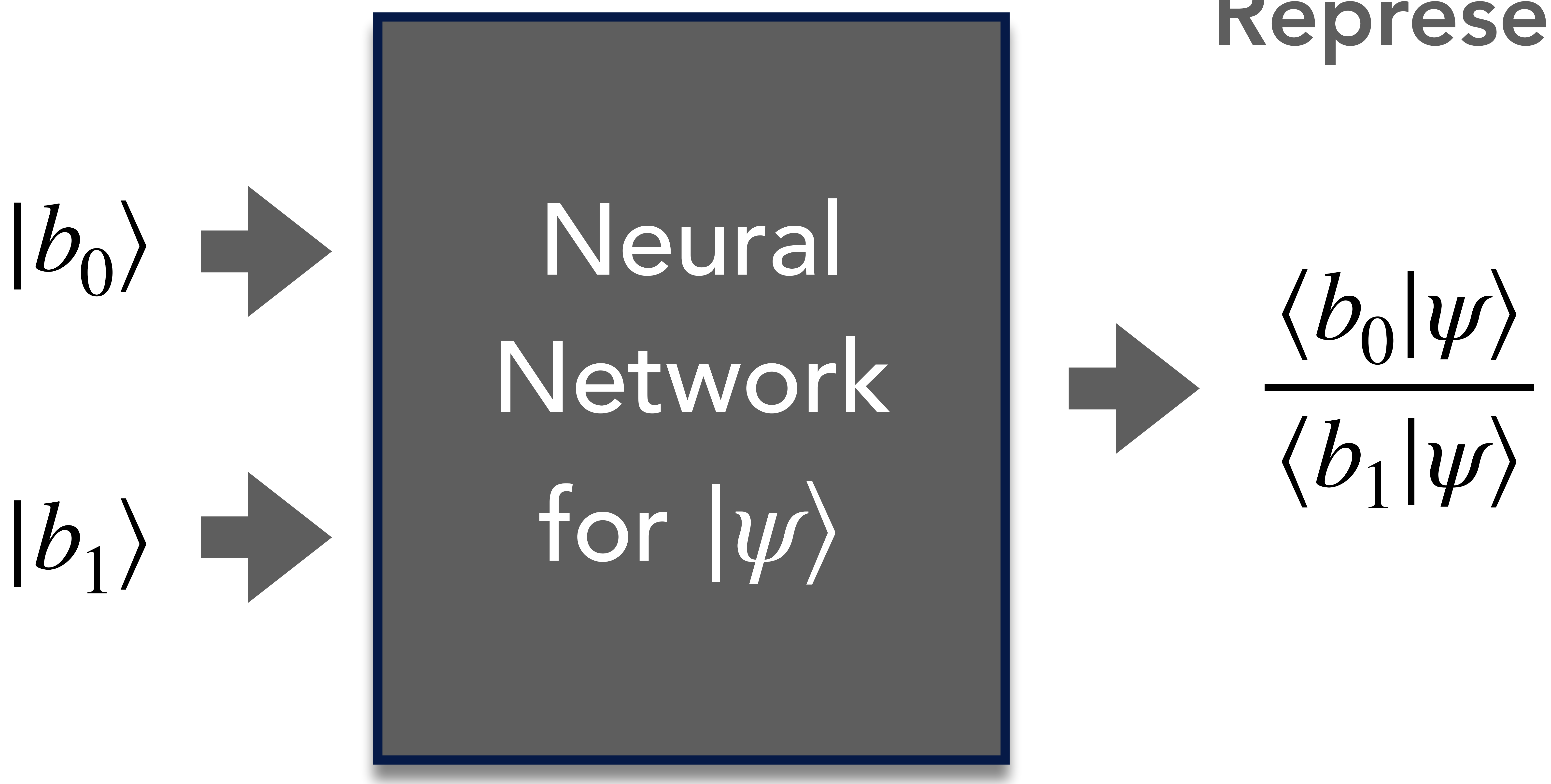
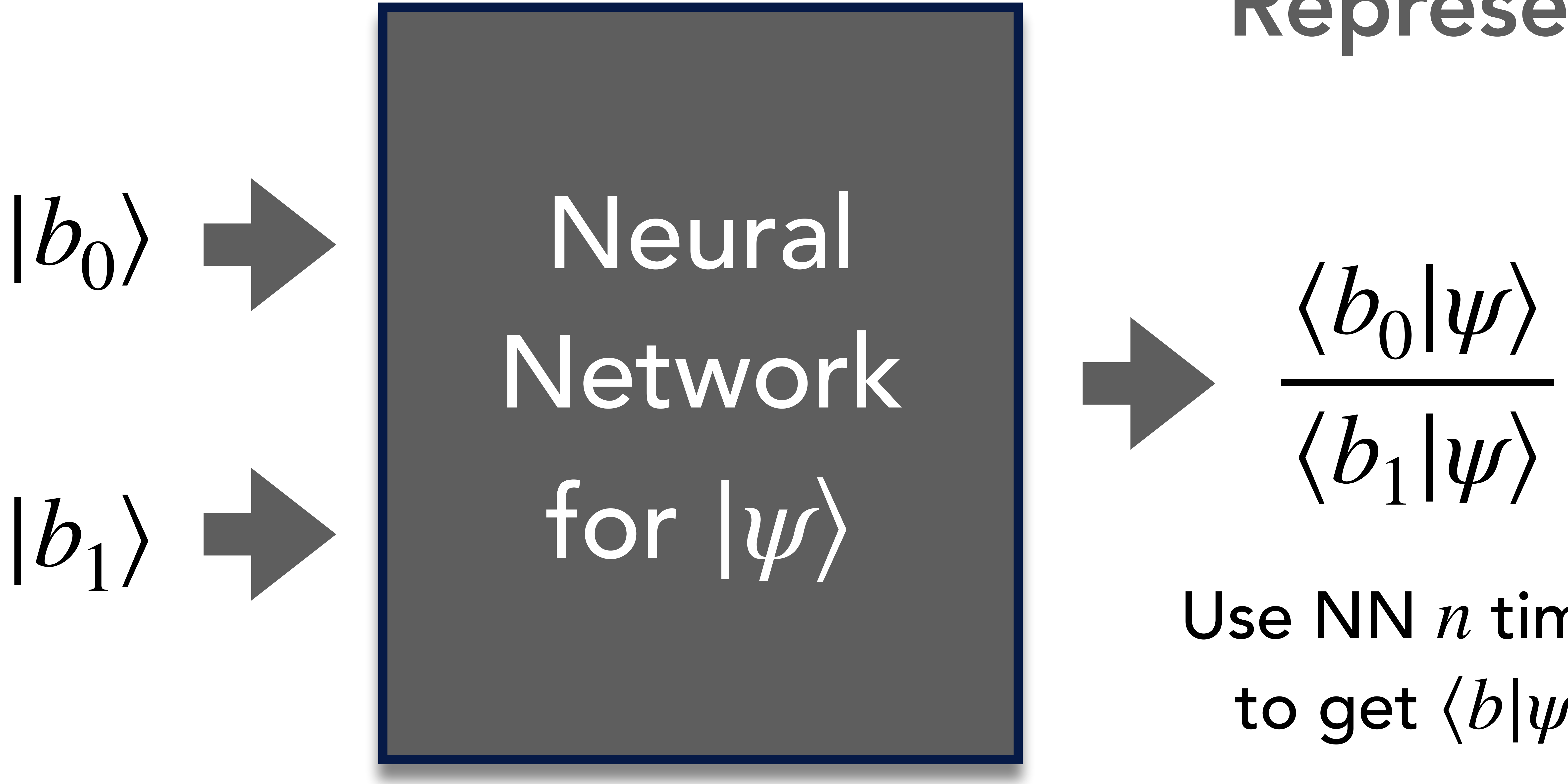


Relative Neural Quantum State

Training/Certifying Neural Q States

Represent $|\psi\rangle$

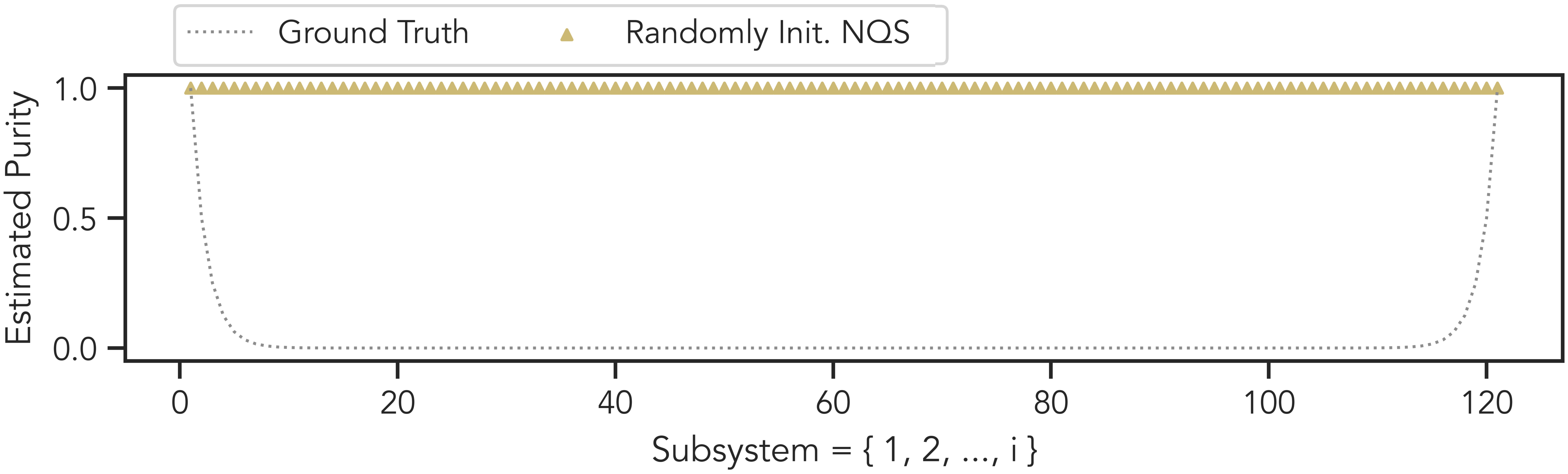


Use NN n times to get $\langle b|\psi\rangle$

Relative Neural Quantum State

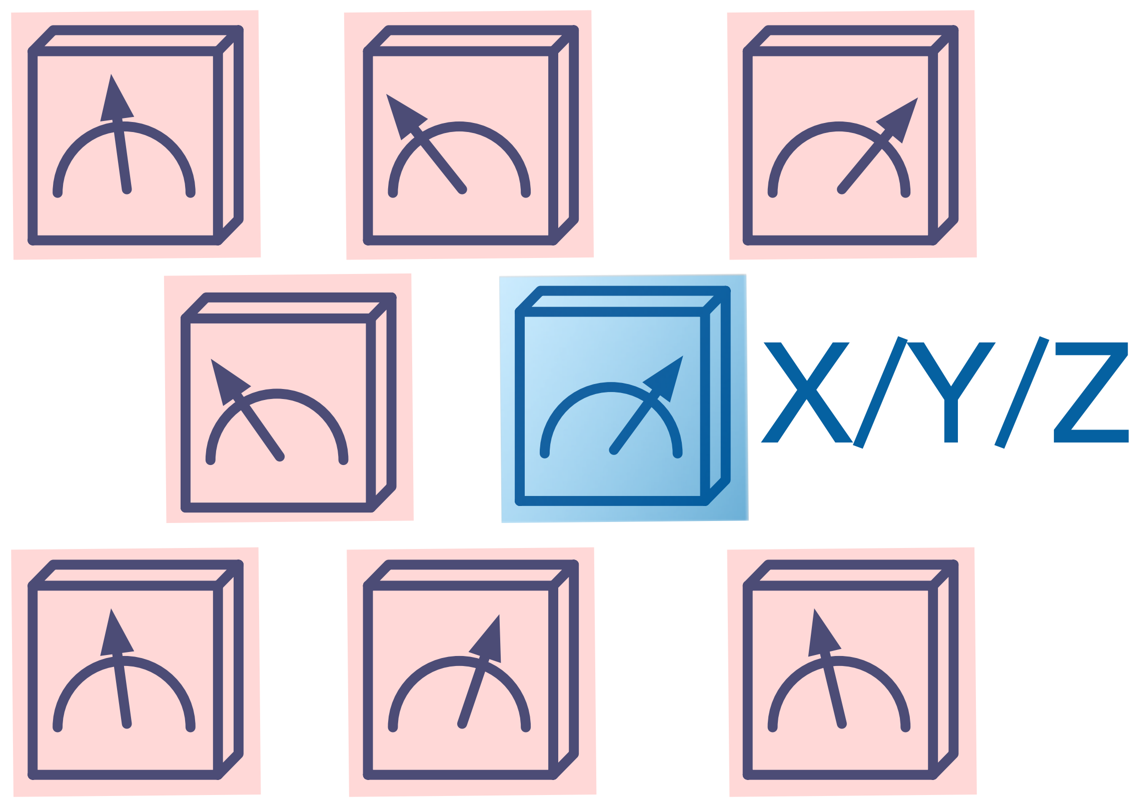
Training/Certifying Neural Q States

We consider learning a class of 120-qubit states with extremely high circuit complexity.

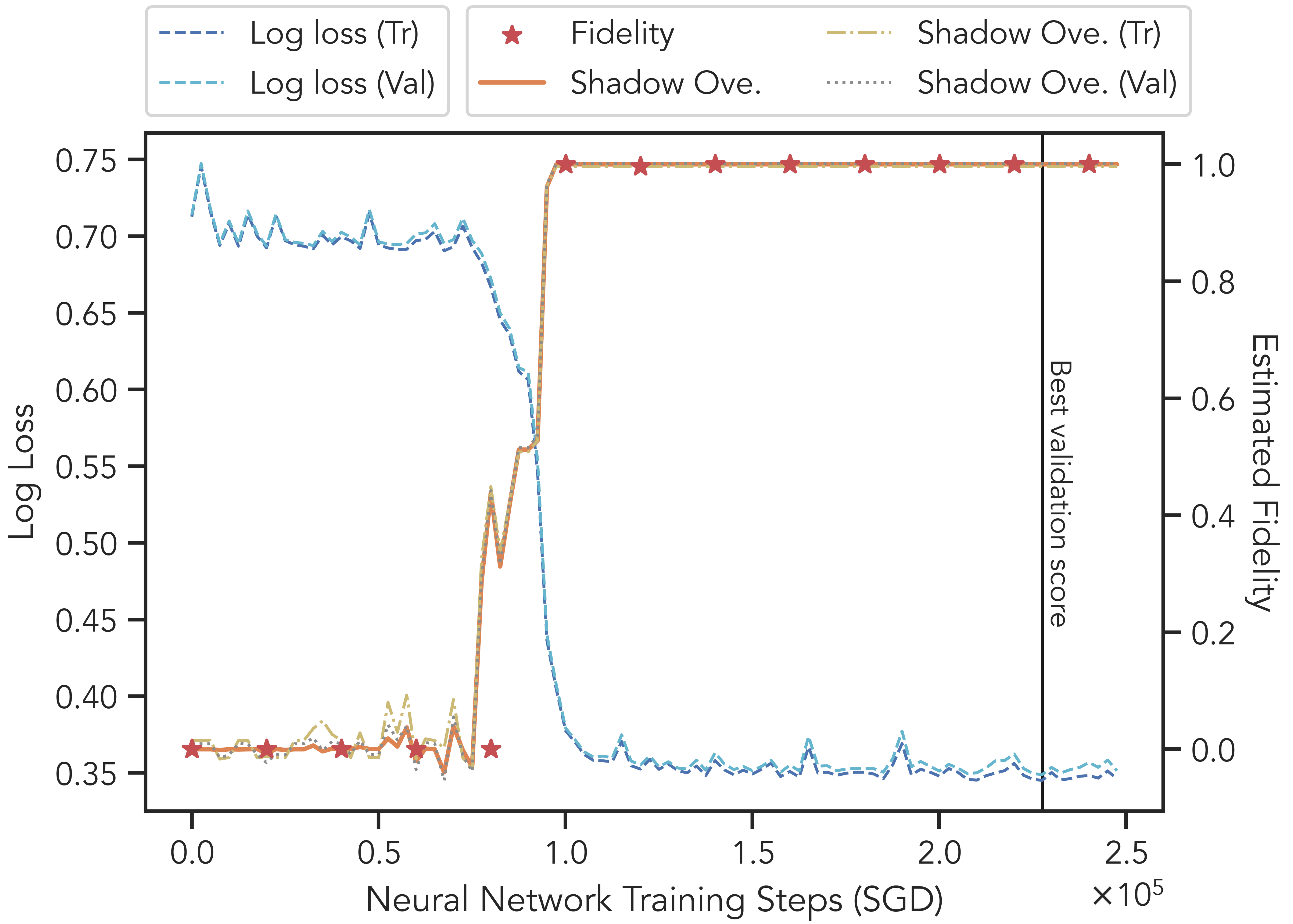


Training/Certifying Neural Q States

Trained using shadow-overlap-based loss



Certified using shadow overlap



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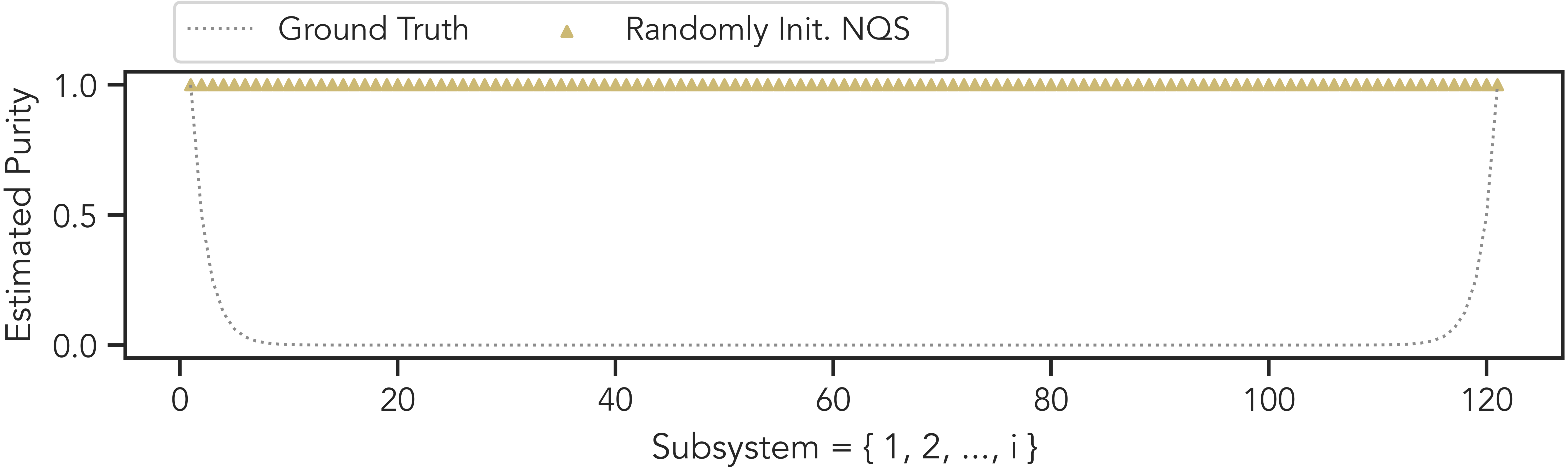

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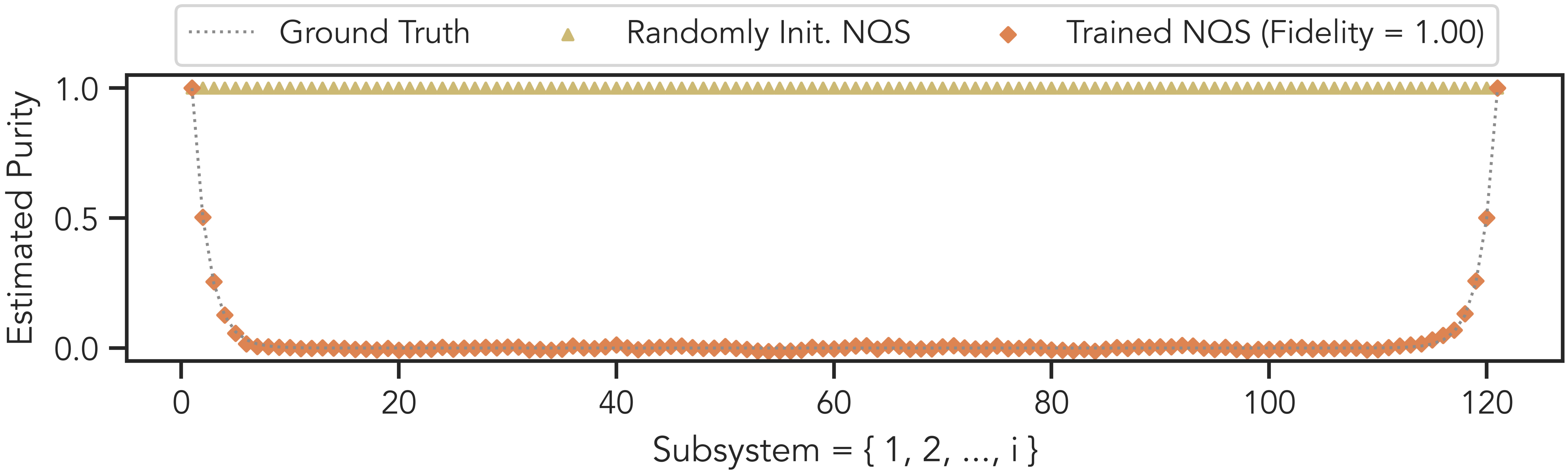


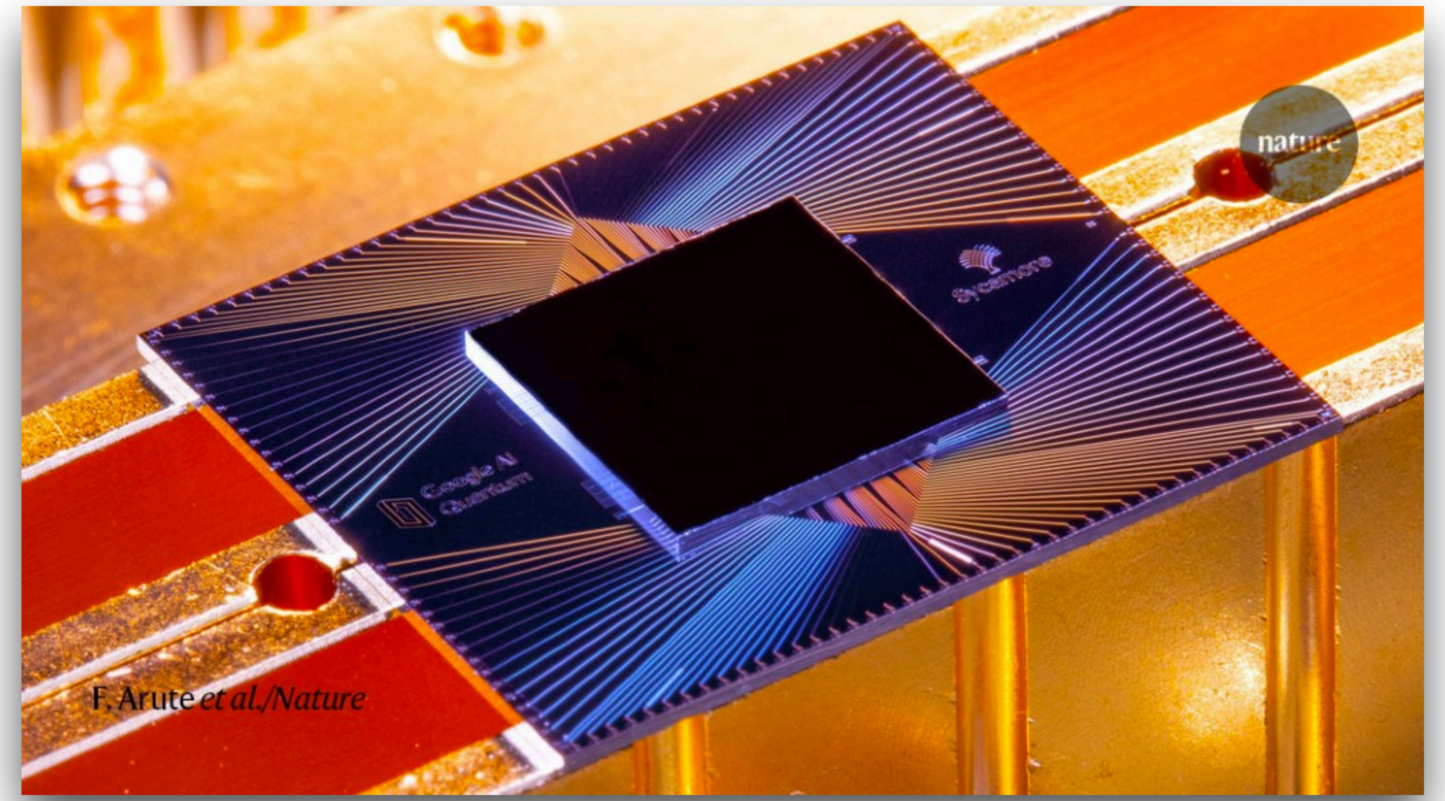
Question: Applications

What can we use state certification for?

Example 1

Benchmarking

Certification enables us to test our quantum devices



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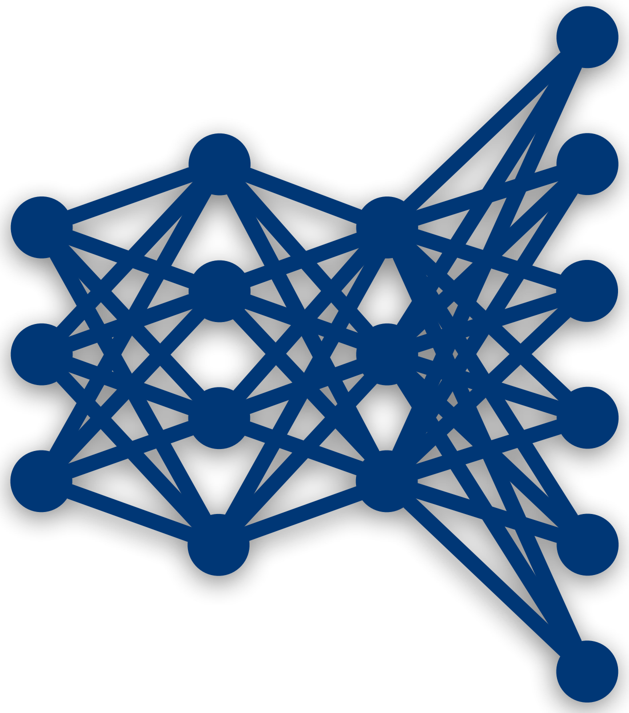

Question: Landscape

How do $\mathbb{E}[\omega]$ vs $\langle\psi|\rho|\psi\rangle$ differ in the following states:

$$|+^n\rangle\langle+^n| \text{ \& } |-^n\rangle\langle-^n|?$$

$$|+^{n-1}-\rangle\langle+^{n-1}-| \text{ \& } |-^n\rangle\langle-^n|?$$

$$|+^{n-k}-^k\rangle\langle+^{n-k}-^k| \text{ \& } |-^n\rangle\langle-^n|?$$

$$\mathbb{E}[\omega] = \frac{1}{n}\sum_{i=1}^{n}\sum_{b_{\neq i}\in\{0,1\}^{n-1}} \mathrm{Tr}\left(\langle b_{\neq i}|\rho|b_{\neq i}\rangle \frac{\langle b_{\neq i}|\psi\rangle\langle\psi|b_{\neq i}\rangle}{\mathrm{Tr}\langle b_{\neq i}|\psi\rangle\langle\psi|b_{\neq i}\rangle}\right) = \mathrm{Tr}\left(L_{|\psi\rangle}\cdot\rho\right) \in [0,1]$$

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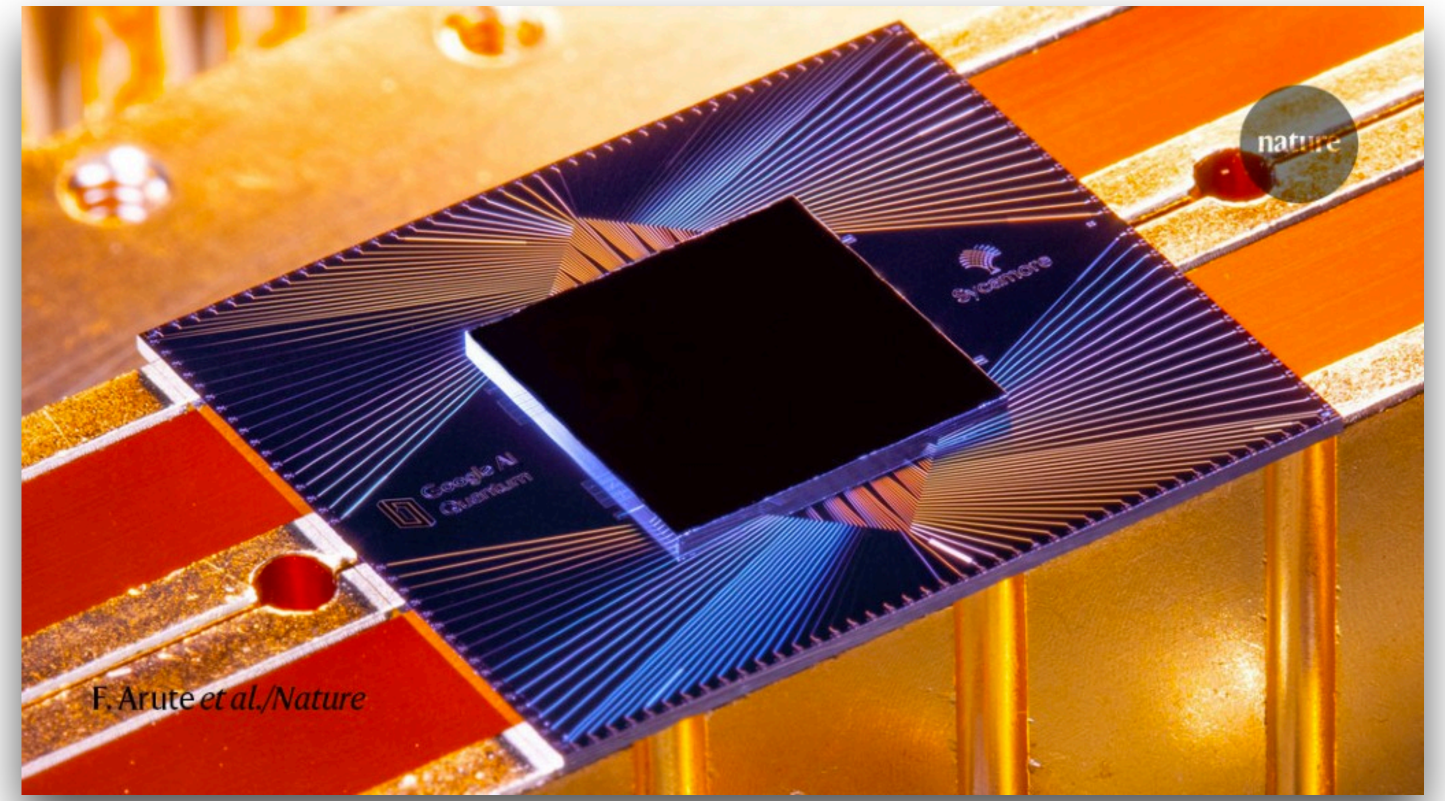

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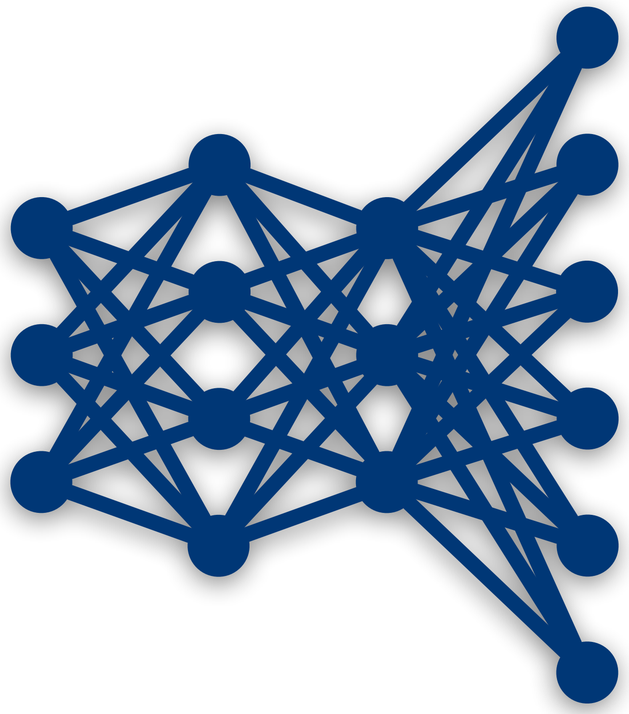

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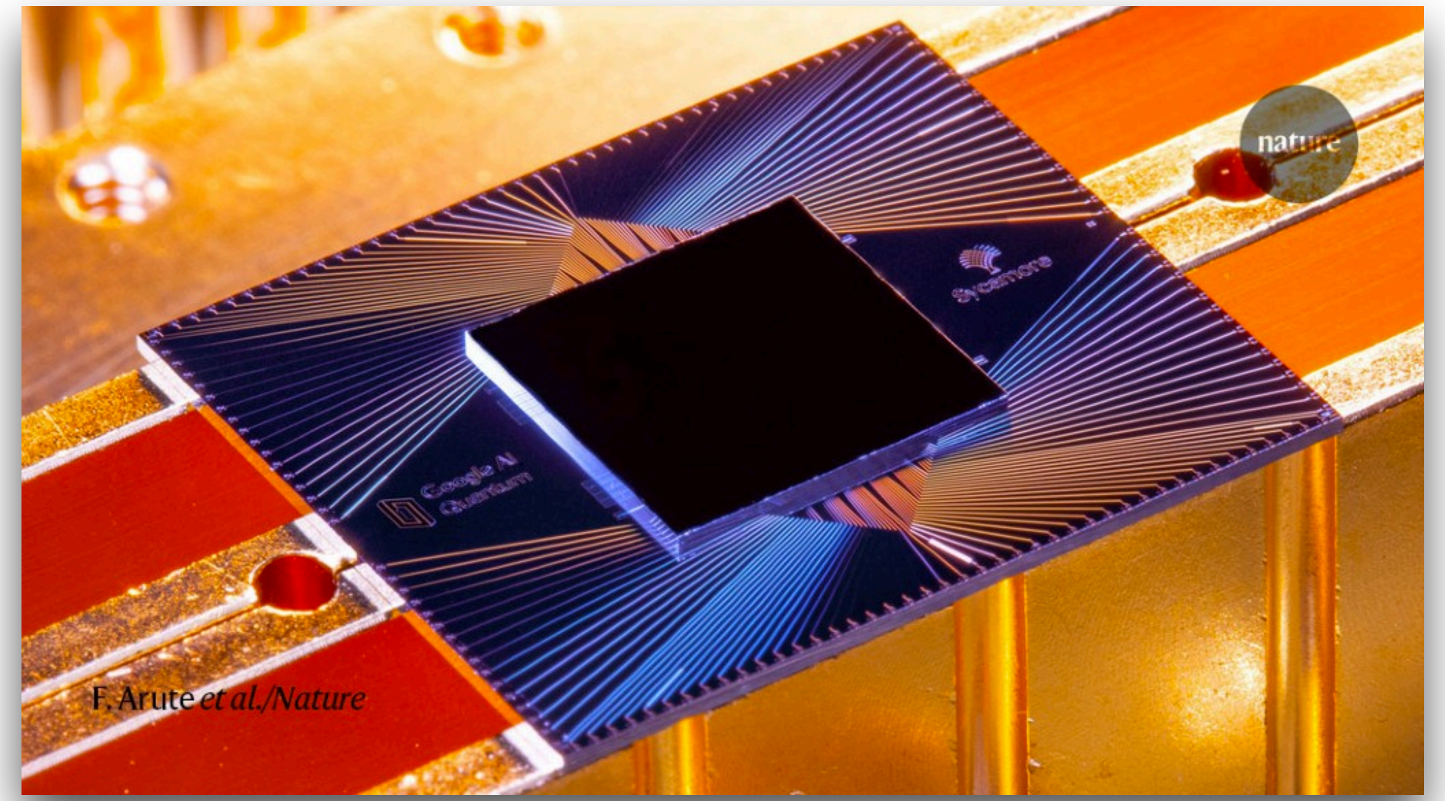

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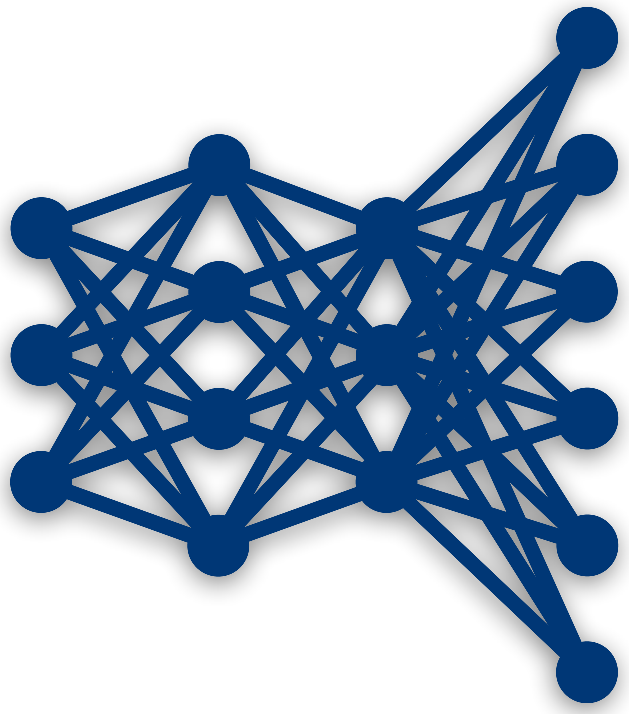
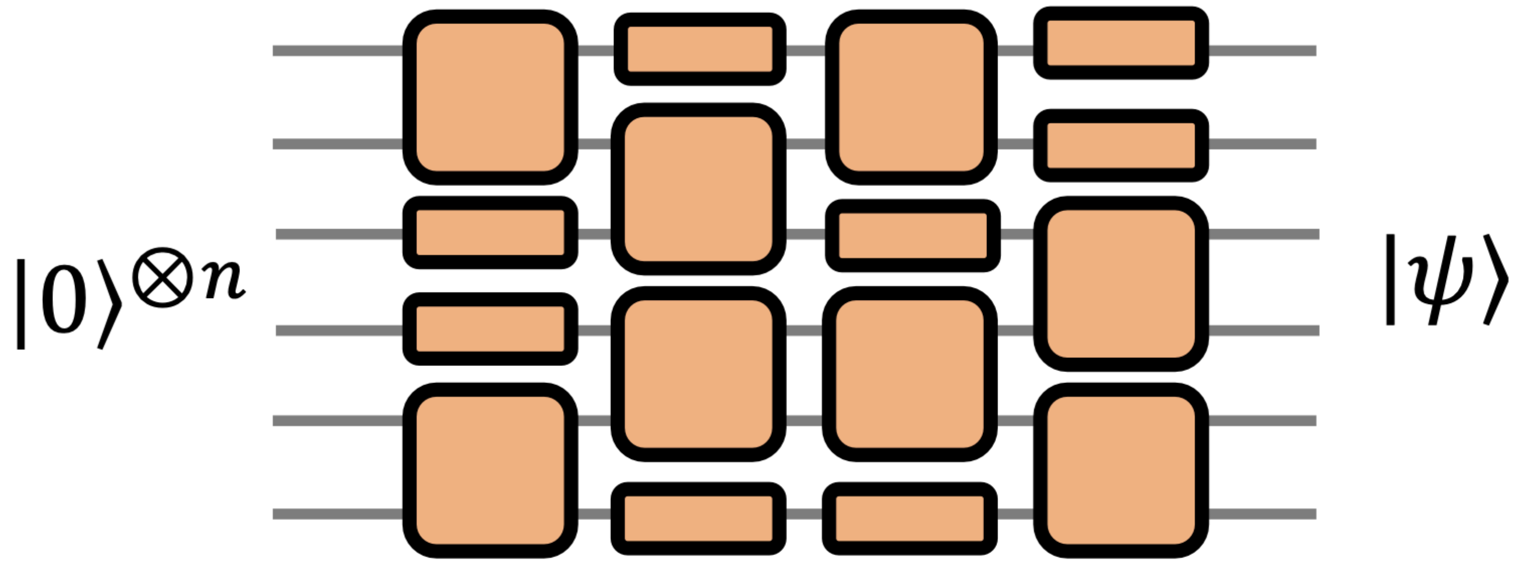


Example 3

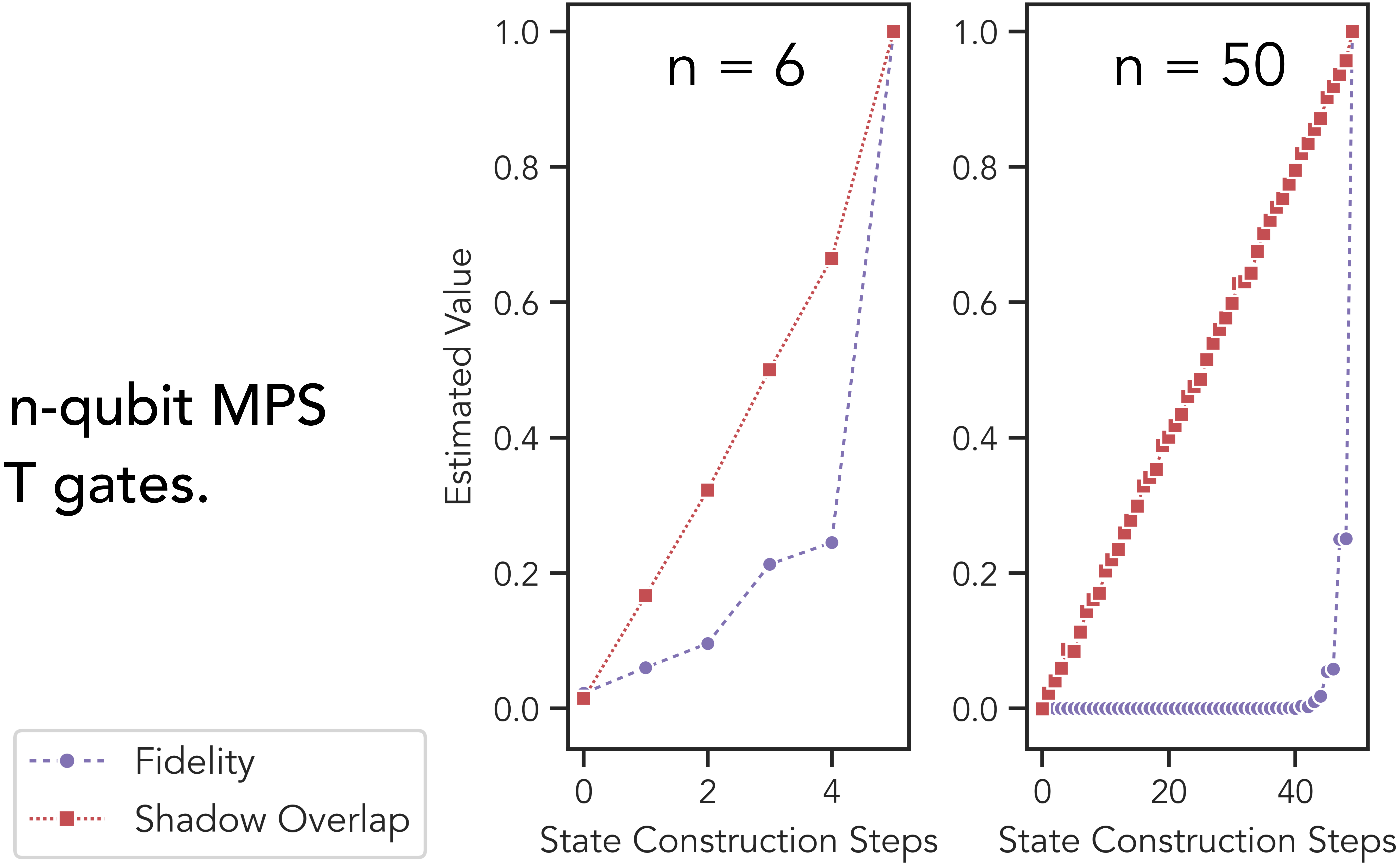
Optimizing circuits

To prepare a target state $|\psi\rangle$, we can optimize the circuit to max the certifier.



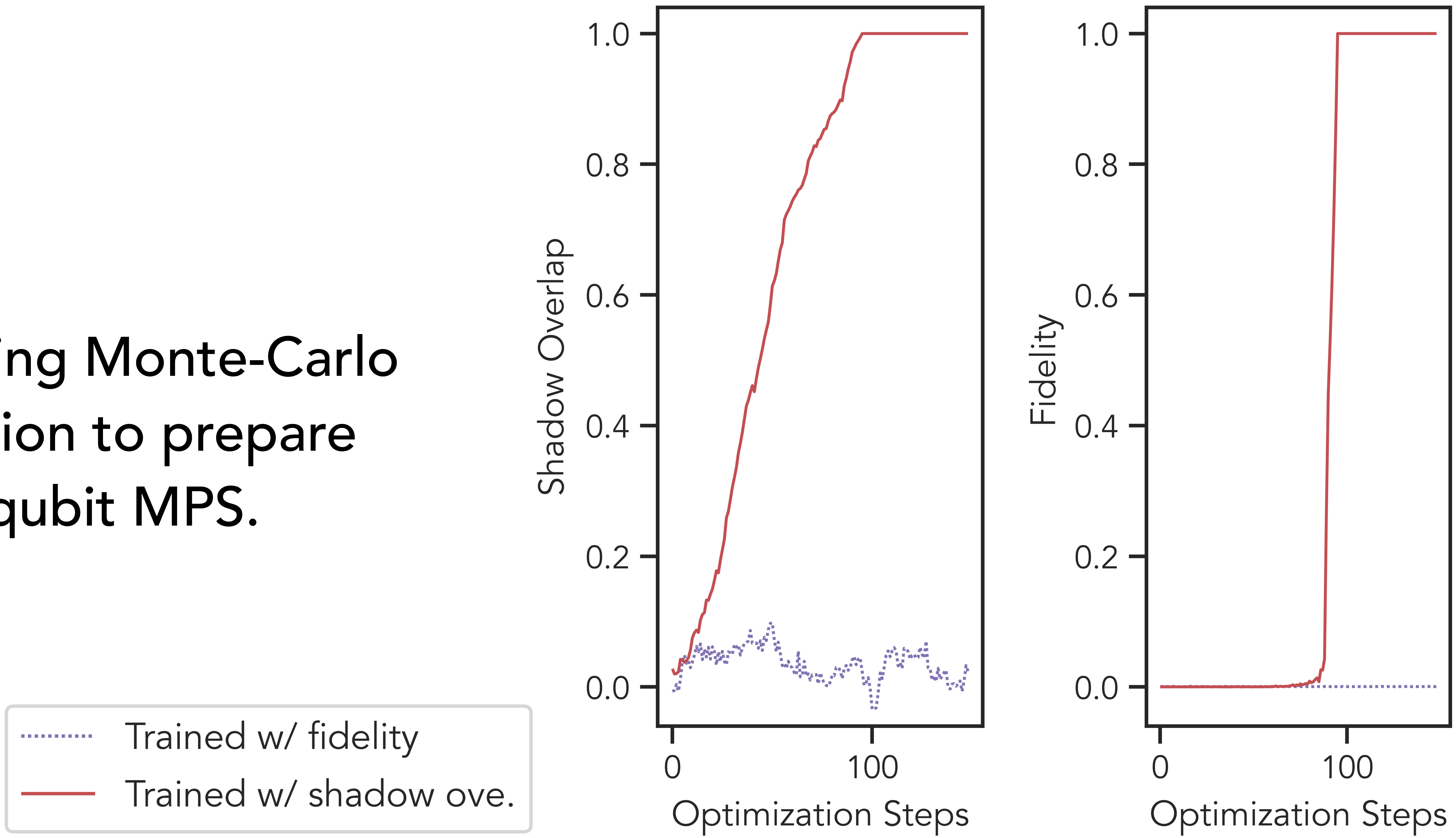
Optimizing state-preparation circuit

Constructing an n-qubit MPS
with H, CZ, T gates.



Optimizing state-preparation circuit

Training using Monte-Carlo optimization to prepare a 50-qubit MPS.



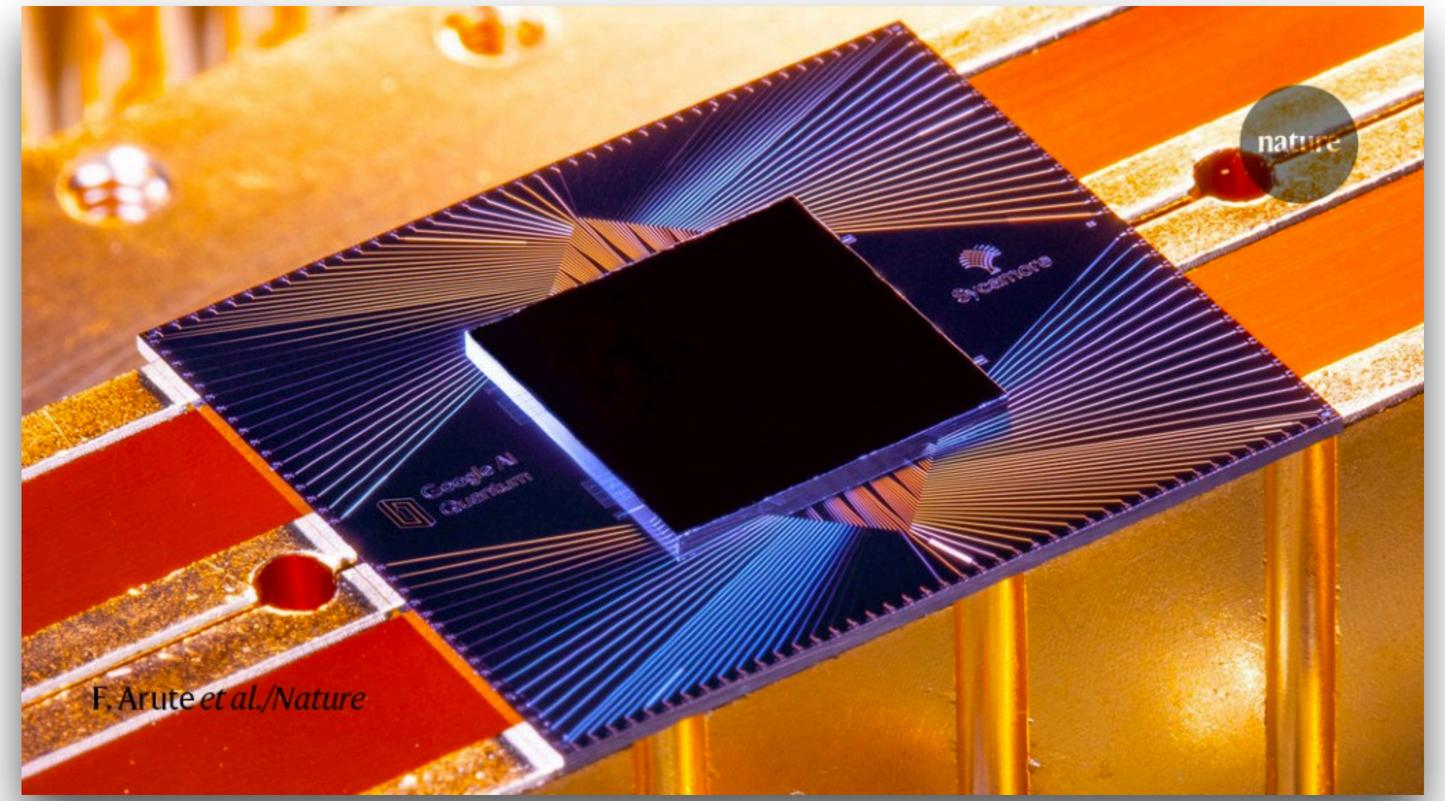
Applications

What can we use this new certification protocol for?

Example 1

Benchmarking

Shadow overlap $\mathbb{E}[\omega]$ certifies if the state has a high fidelity



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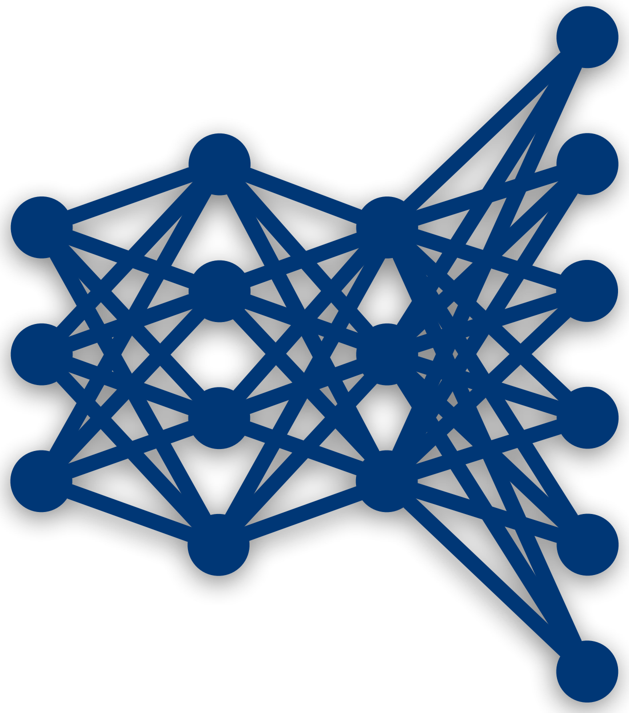

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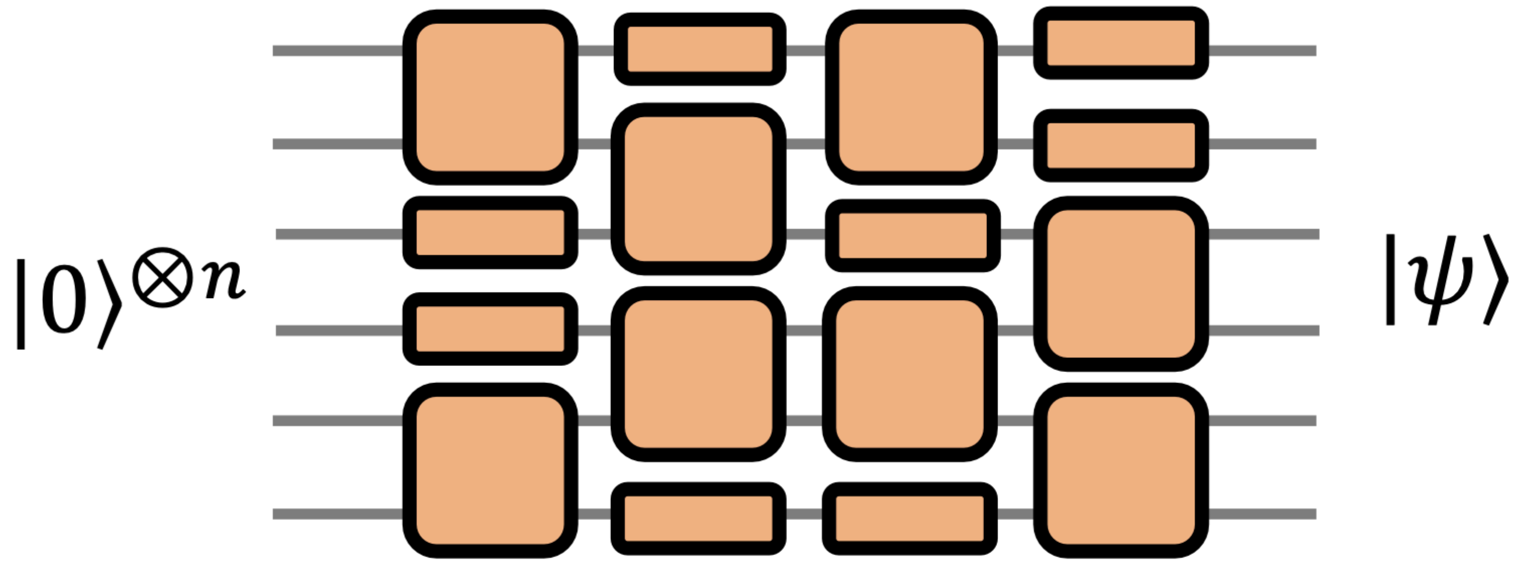
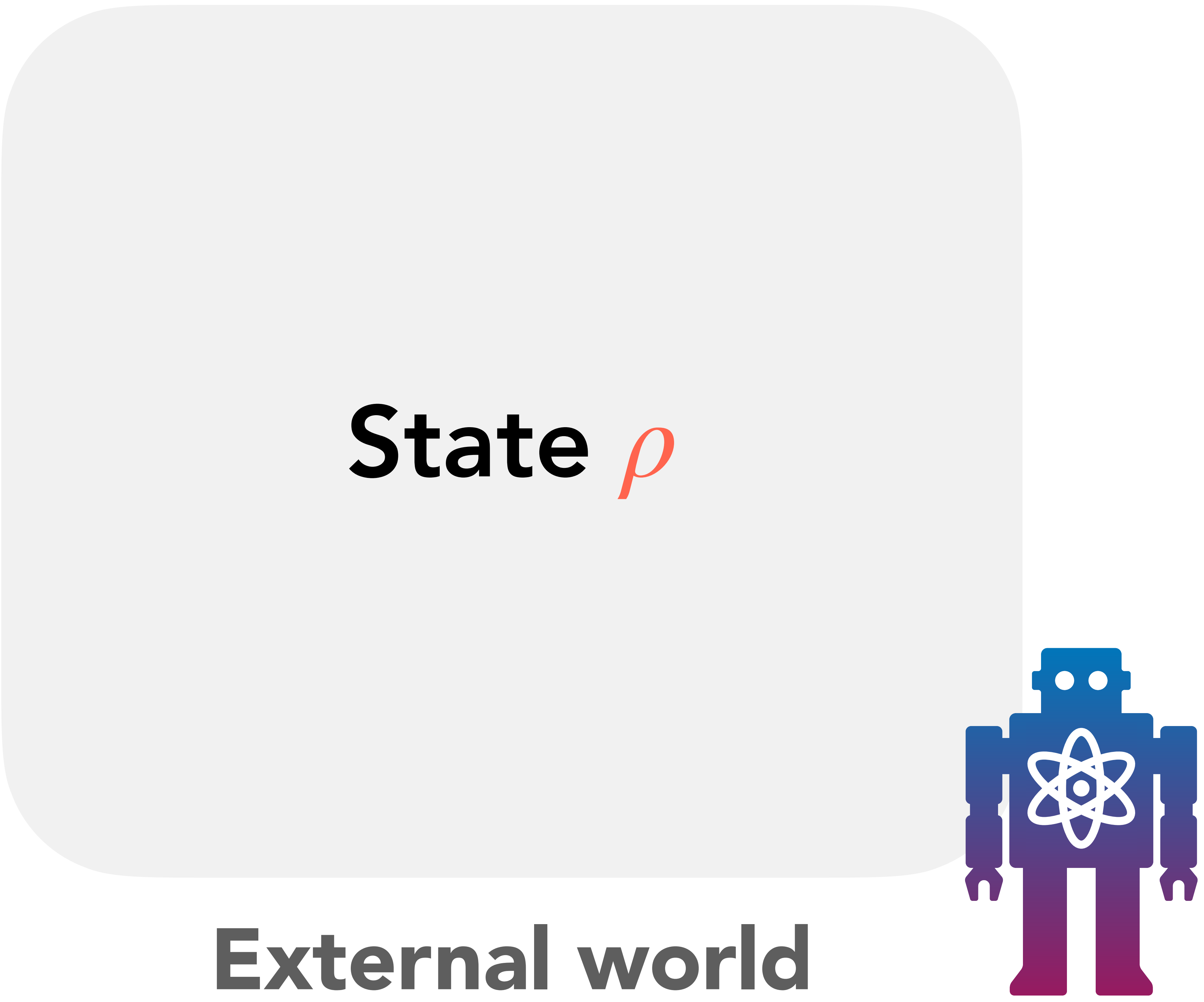


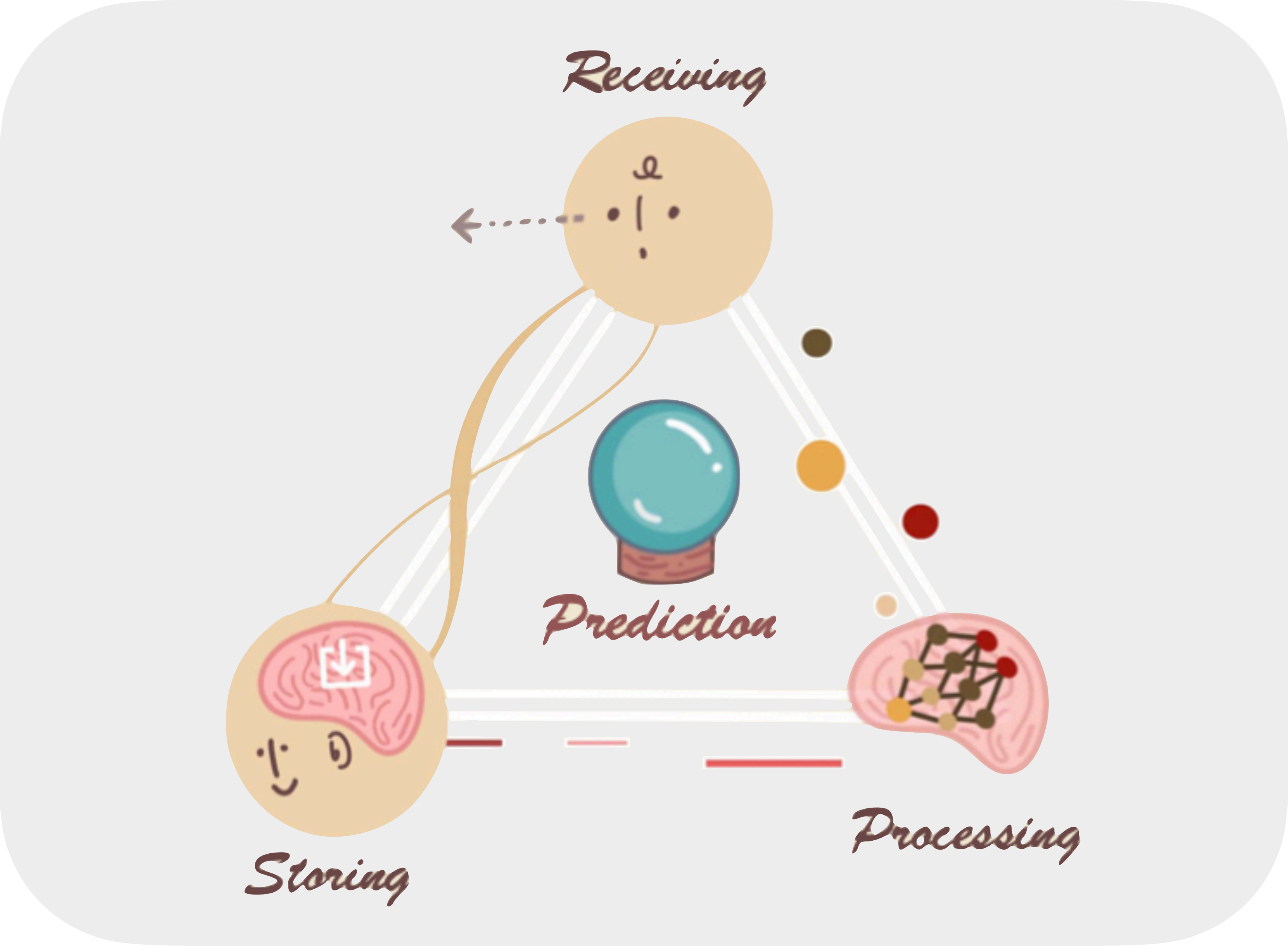
Question: Ultimate Certifier

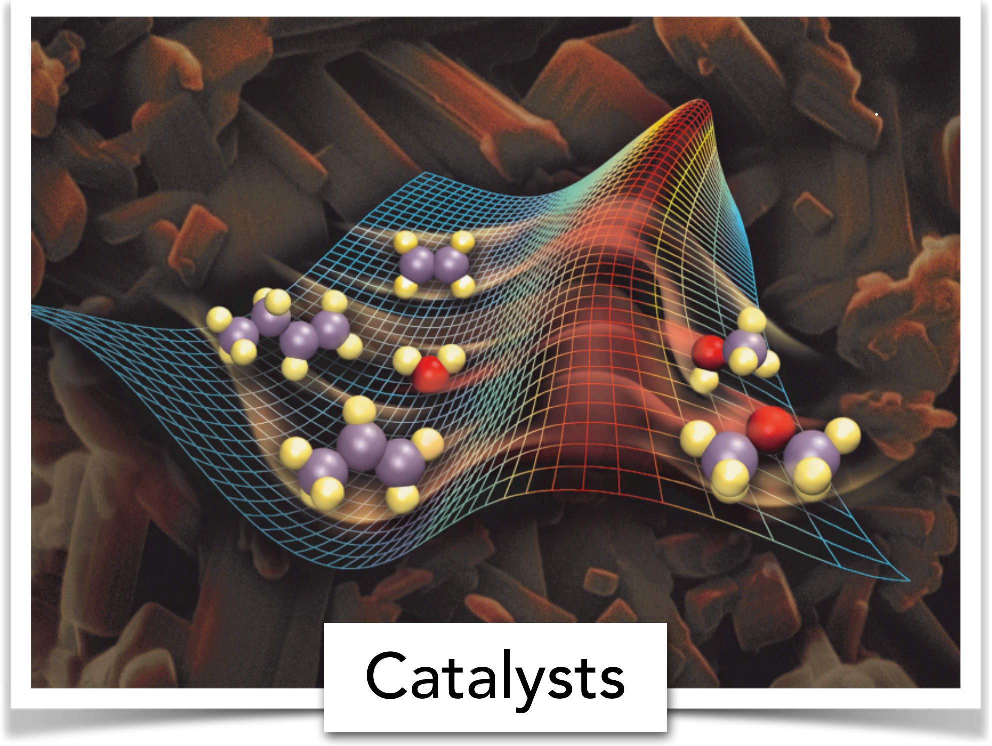


Can we efficiently certify **any** state $|\psi\rangle$ w/ few single-qubit measurements?

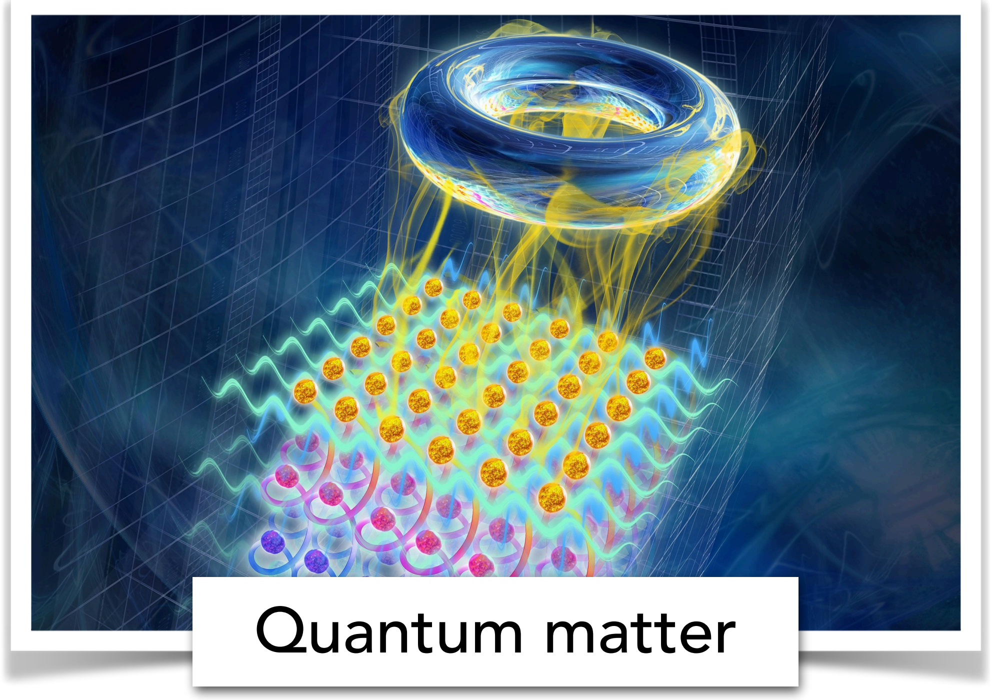
Conclusion

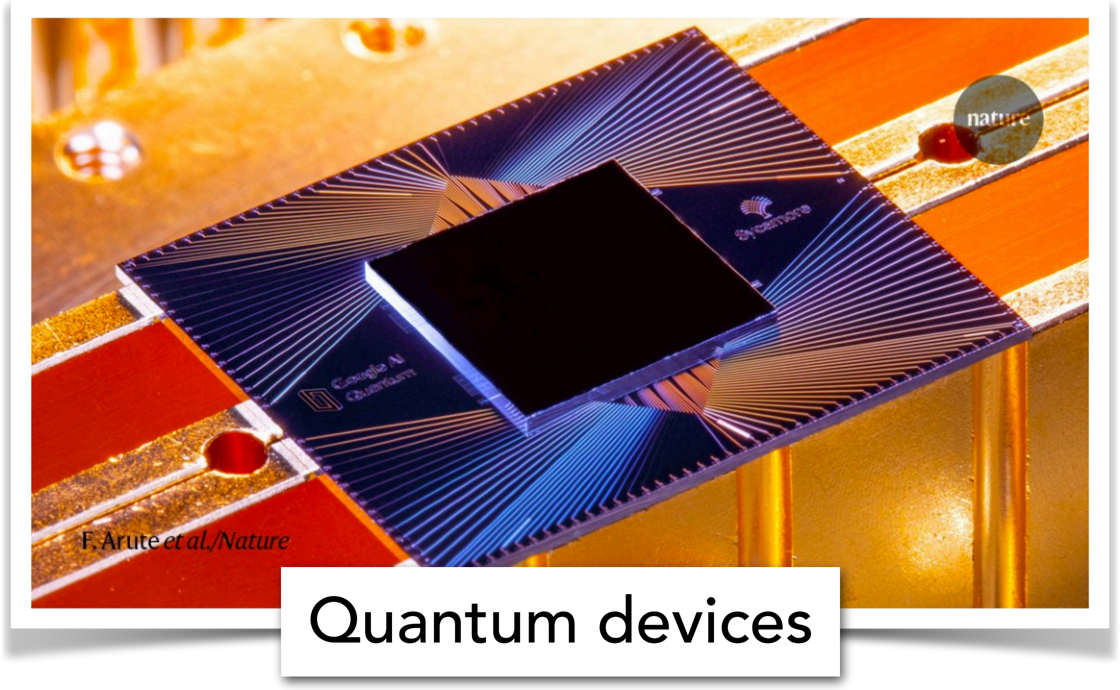
- To accelerate/automate quantum science, it is critical to understand how to design better algorithms to learn in the quantum universe.




Catalysts


Pharmaceutics


Quantum matter

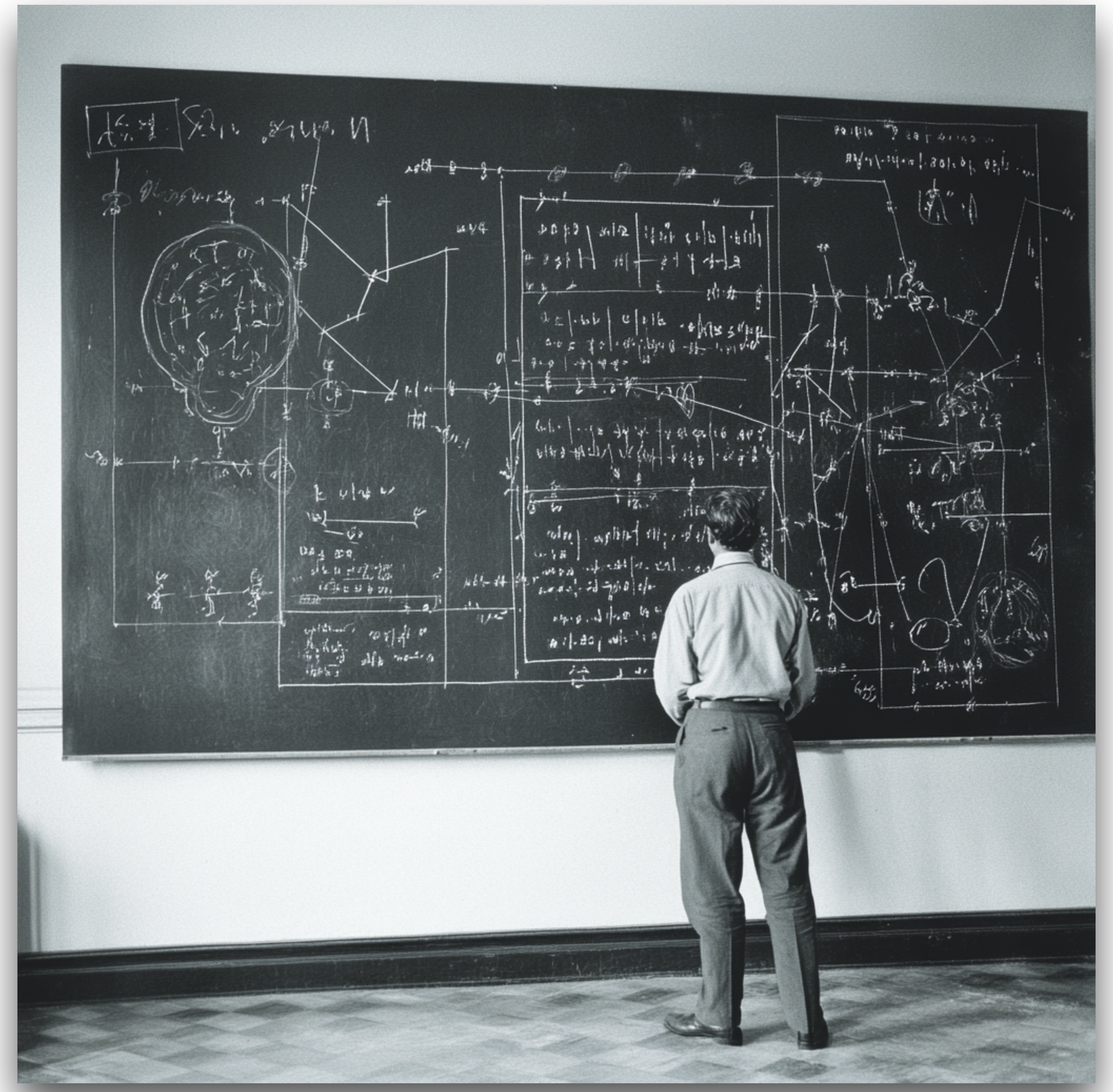


Quantum devices

Image credits: (Top left) https://www.energy.gov/science/doe-explainscatalysts (Top right) https://theconversation.com/as-pharmaceutical-use-continues-to-rise-side-effects-are-becoming-a-costly-health-issue-105494 (Bottom left) https://news.mit.edu/2019/ultra-quantum-matter-uqm-research-given-8m-boost-0529 (Bottom right) https://www.nature.com/articles/d41586-019-03213-z

Conclusion

- Powerful learners (humans/machines) have **emergent capabilities** that are inherently heuristics—unpredictable by first principle.



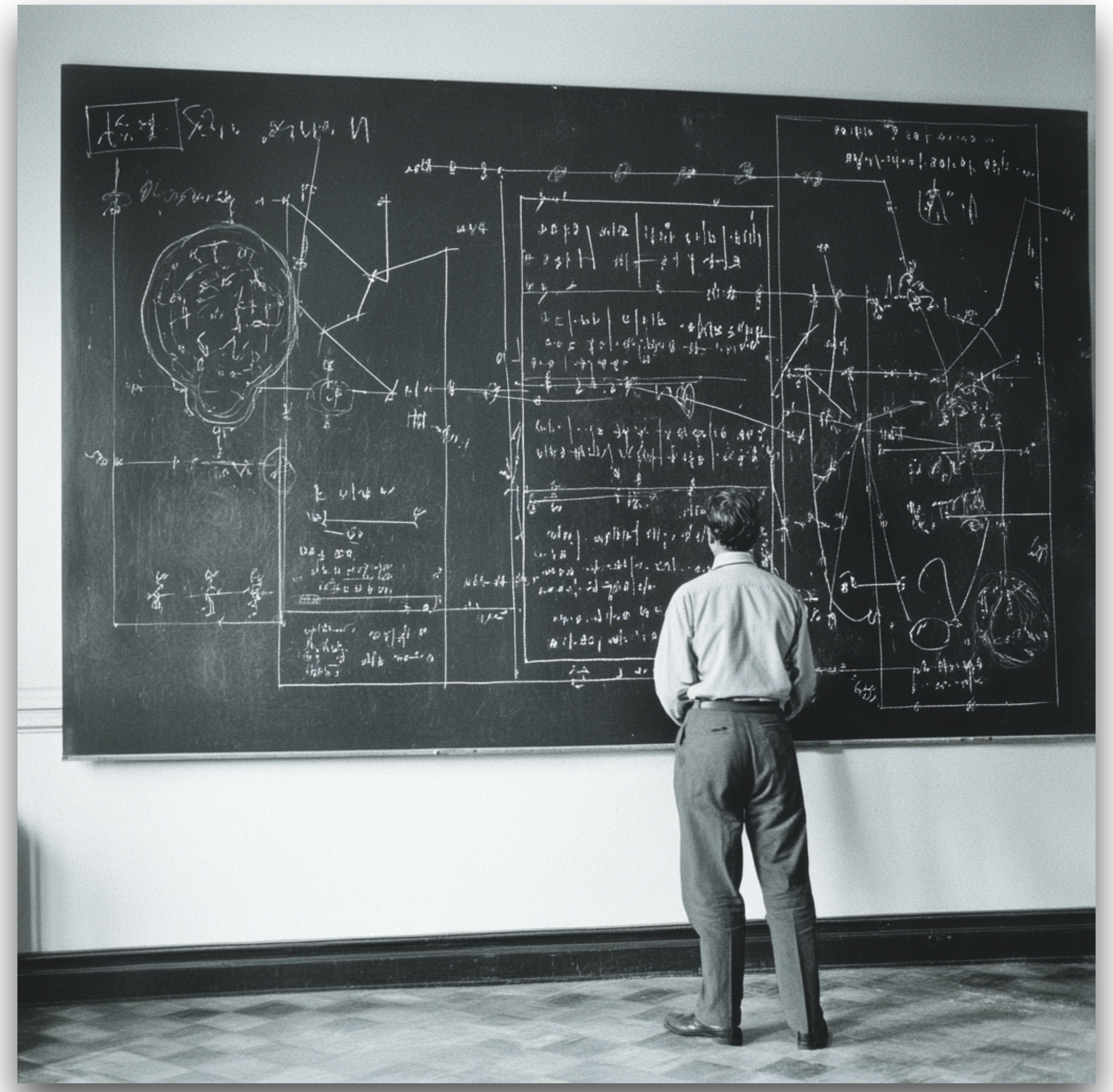
Theorists dreaming

Experimentalists building

AI analyzing

Conclusion

- How to design rigorous certification protocols to harness and validate these empirically powerful but heuristic emergent capabilities?



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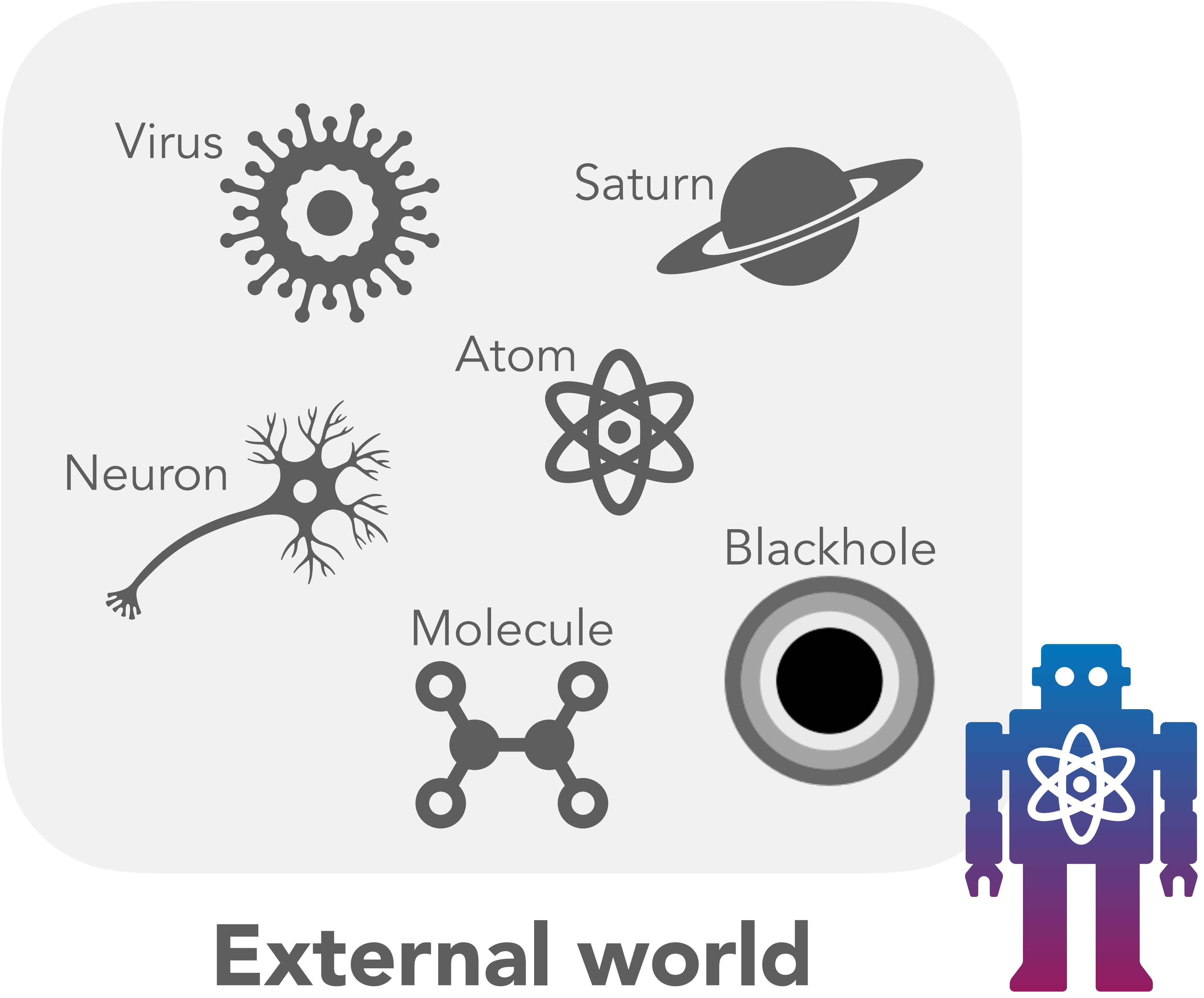
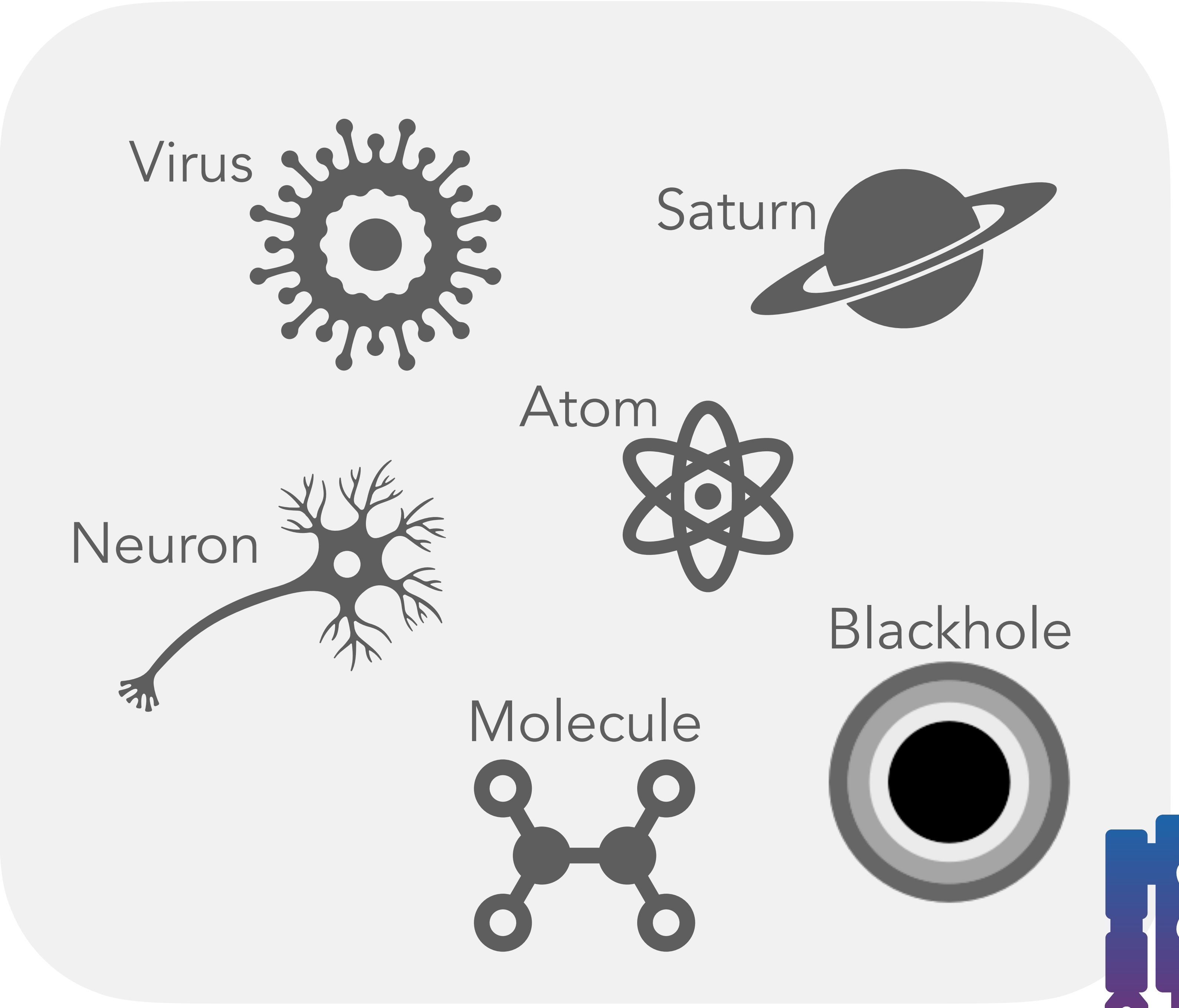


How can a future quantum AI

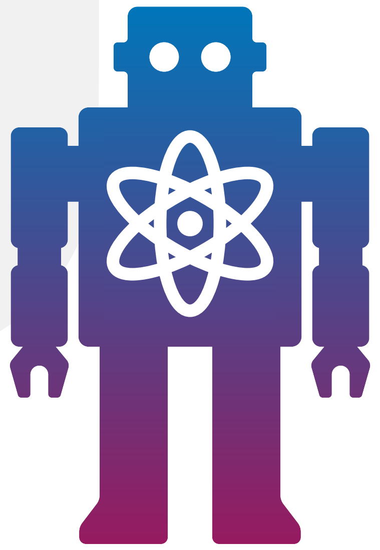
learns models,
extracts properties,
makes predictions,

about the external world?

Certification



External world

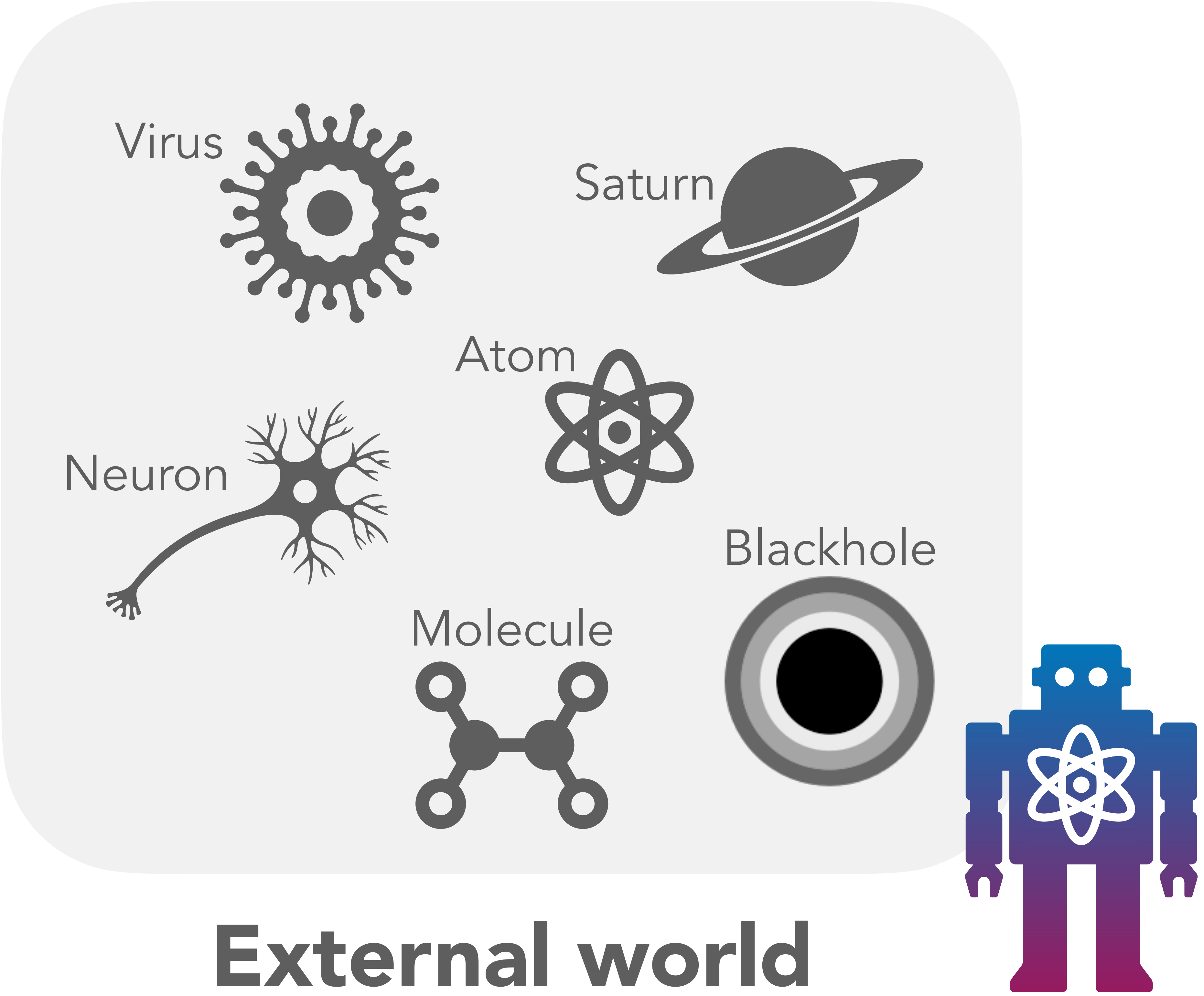


When a future quantum AI

learns models,
extracts properties,
makes predictions,

better than us, how to certify it?

Question: Simulation

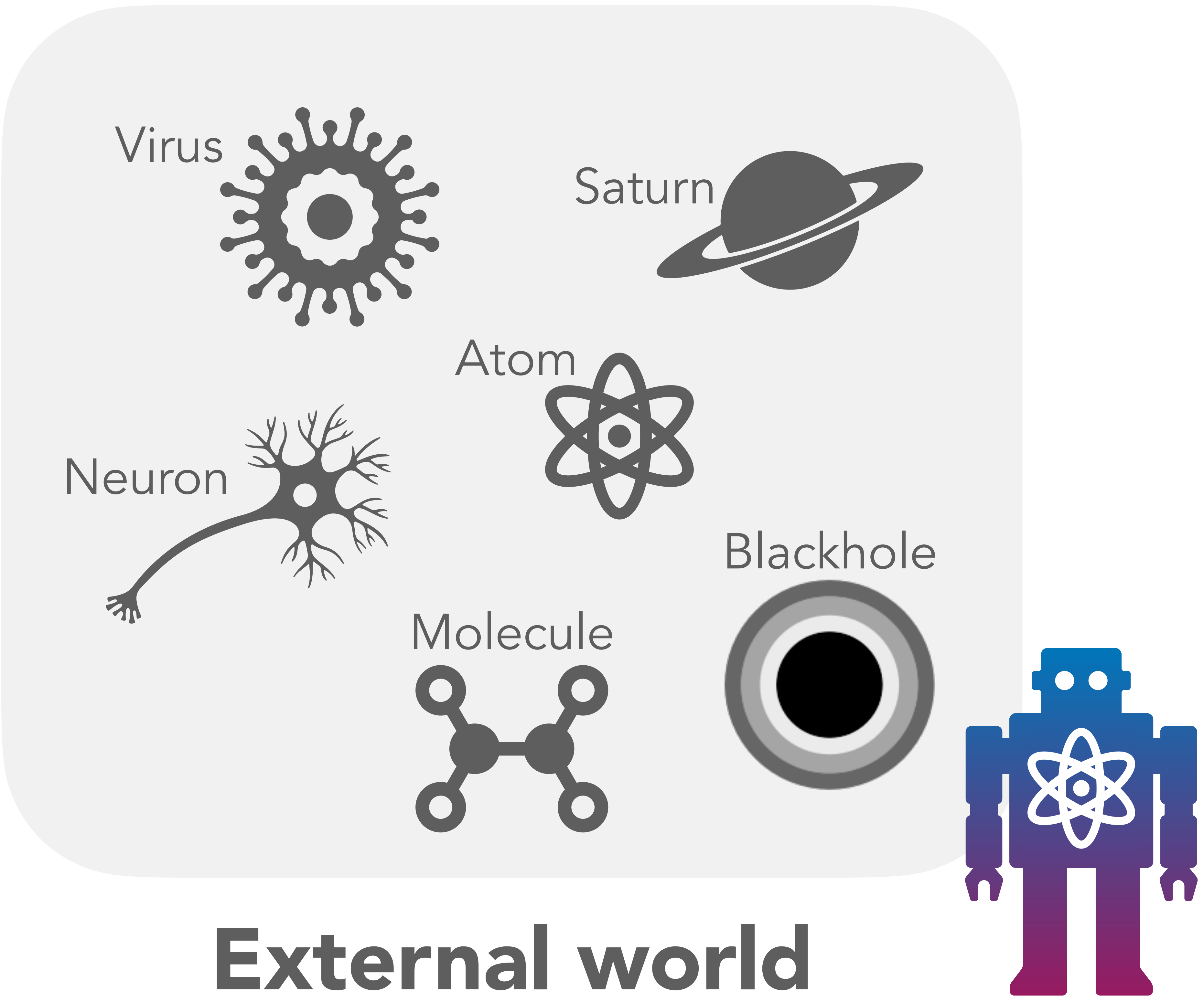


External world

When a future quantum AI says it has found a new low-depth q. circuit for simulating electrons,

how to certify/harness it rigorously?

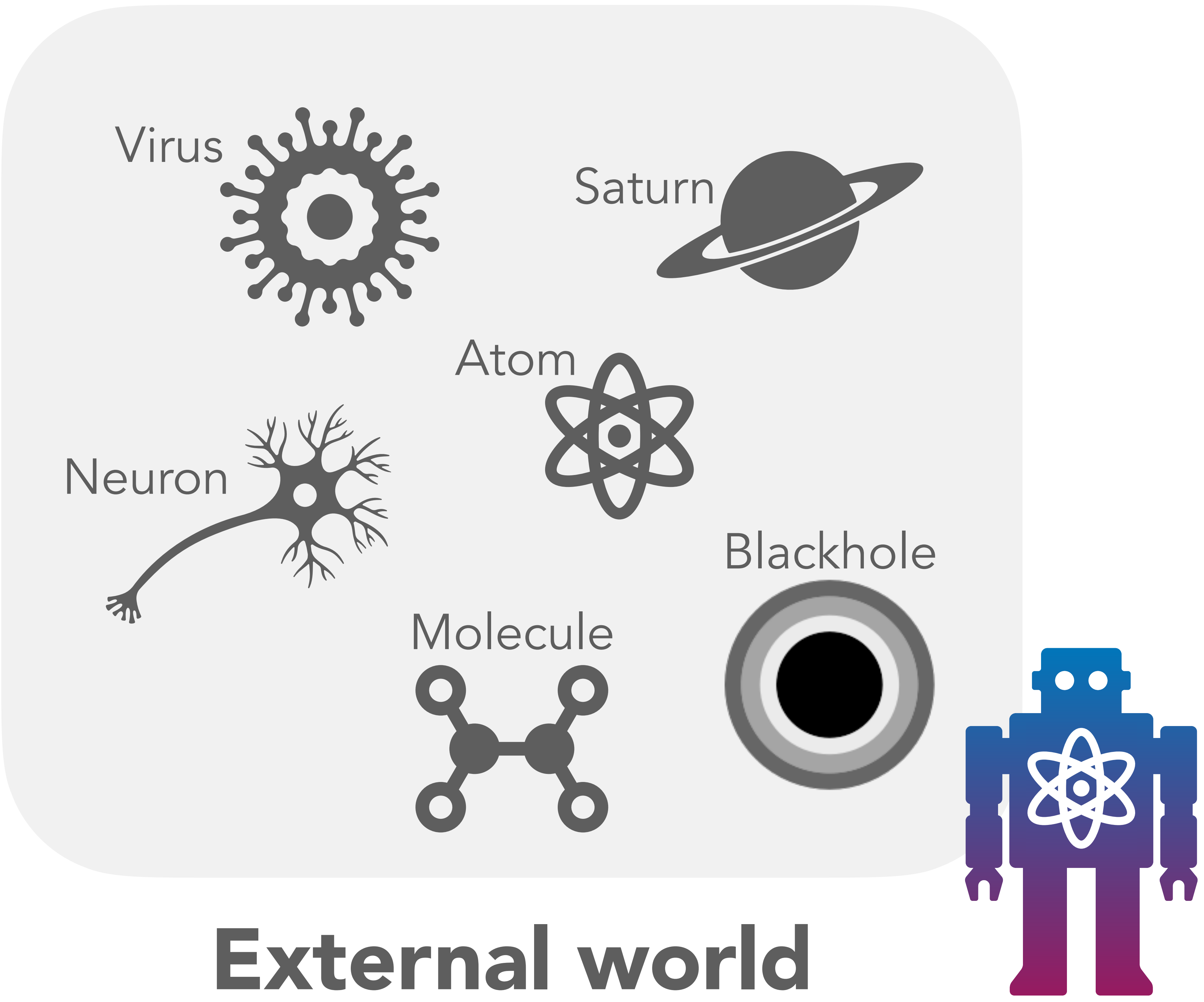
Question: Algorithm



When a future quantum AI says it has designed a new quantum algorithm with genuine quantum advantage,

how to certify/harness it rigorously?

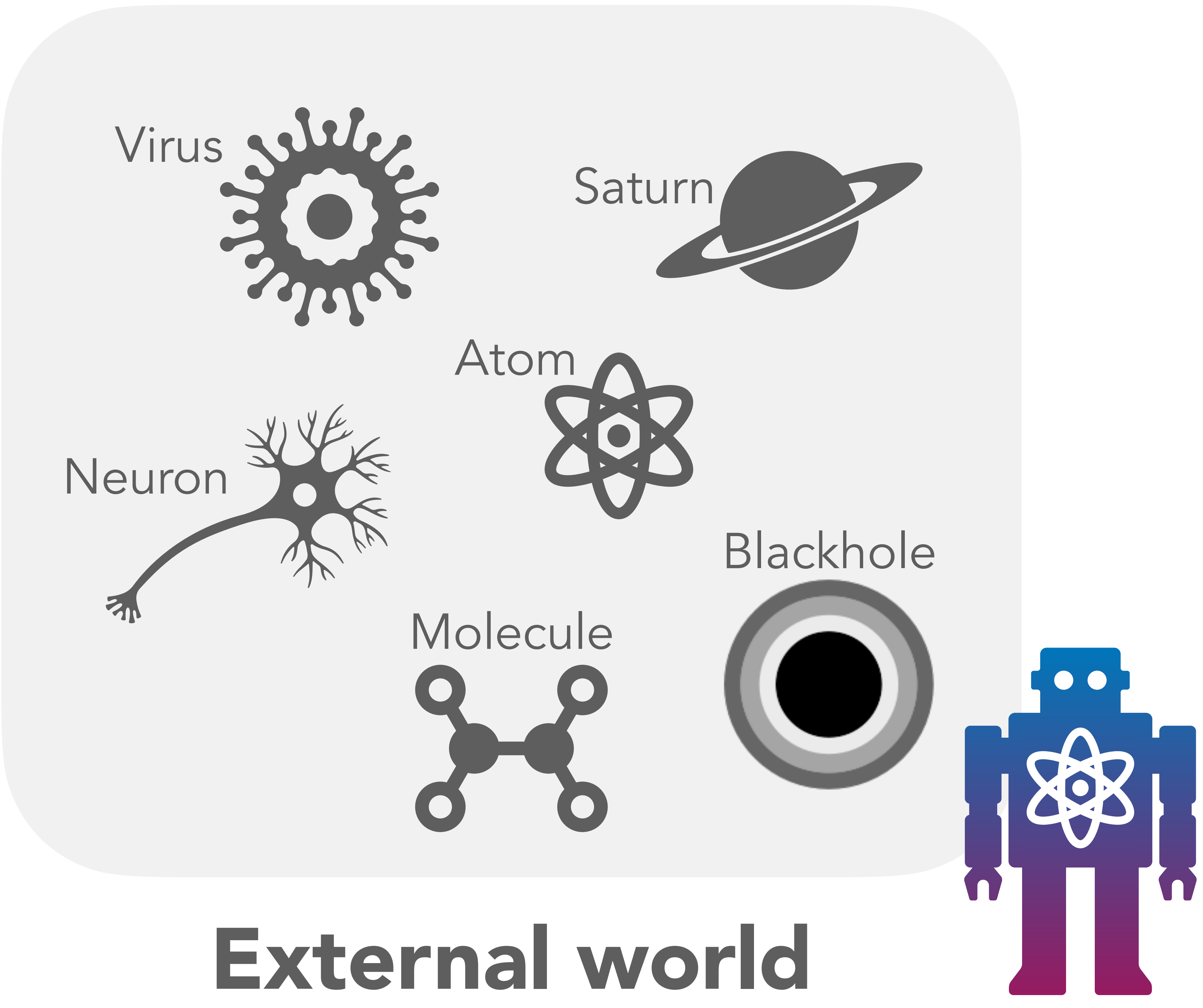
Question: State of Matter



When a future **quantum AI** says it has discovered a new **state of matter**,

how to certify/harness it rigorously?

Question: Sensing



When a future quantum AI says it has sensed axion dark matter,

how to certify/harness it rigorously?

Long-term goals

1. Develop our understanding of **learning** to accelerate/automate science.
2. Create **certification** protocols to validate/harness emergent capabilities.



AI imagination of itself learning and discovering new facets of our quantum universe