

Learning to predict arbitrary quantum processes

Presenter: Hsin-Yuan Huang (Robert)

Joint work with Sitan Chen and John Preskill



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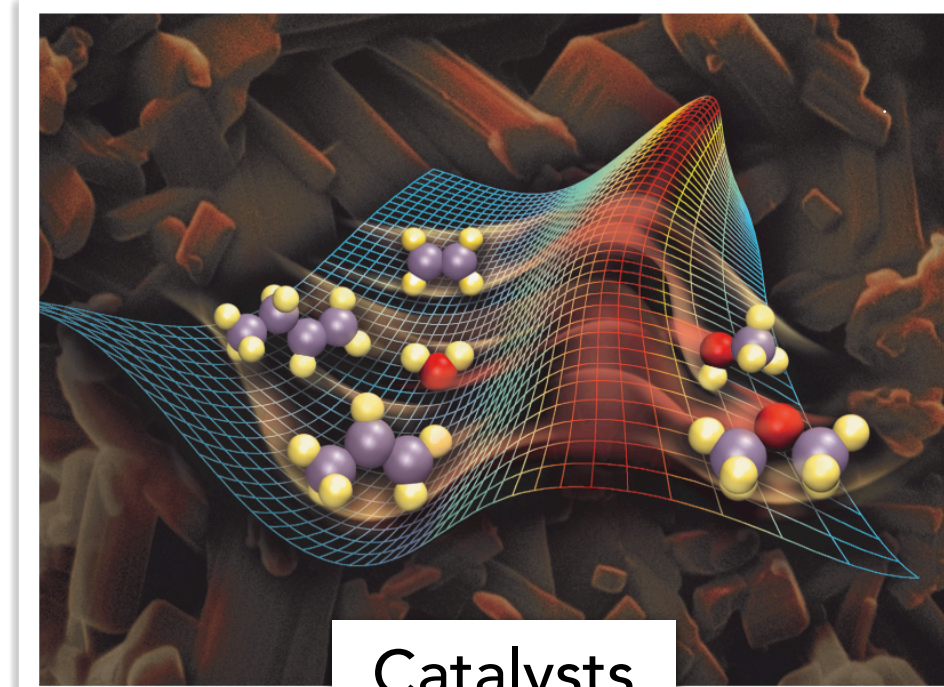
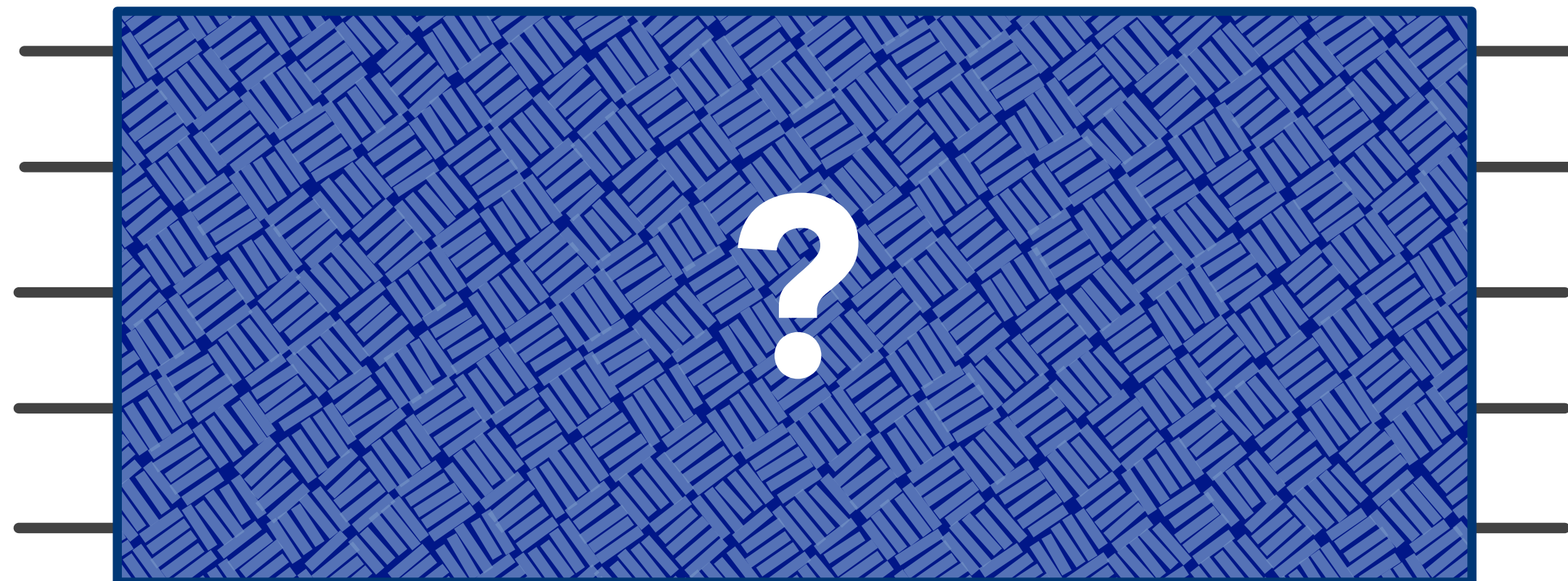
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aws

Motivation

- We have seen substantial recent progress on efficiently learning to predict quantum states.
- Are there efficient algorithms for learning to predict quantum circuits / processes?

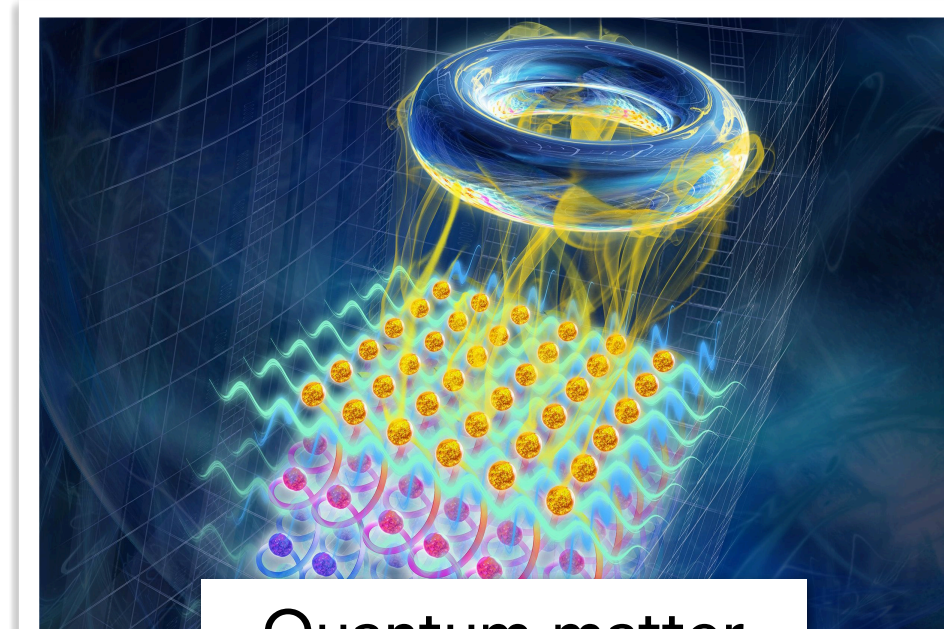
A high-complexity quantum process



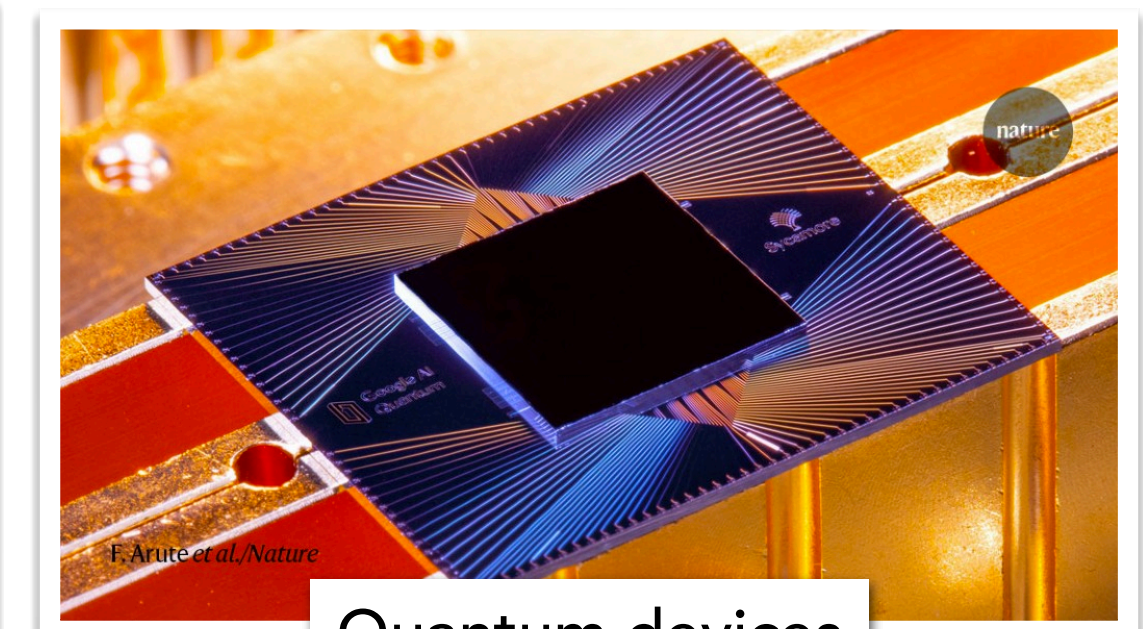
Catalysts



Pharmaceuticals



Quantum matter



Quantum devices

The Setting

- In this work, we focus on training an ML model to learn and predict

$$\rho, O \mapsto f_{\mathcal{E}}(\rho, O) = \text{Tr}(O\mathcal{E}(\rho)),$$

where ρ is an input quantum state, \mathcal{E} is an (unknown) CPTP map, and O is an observable.

- This includes any function computable by a quantum computer (in exponential time).

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Example 1

*Predicting outcomes of
physical experiments*

ρ : initial state given by classical input x

\mathcal{E} : the physical process in the experiment

O : what the scientist measure



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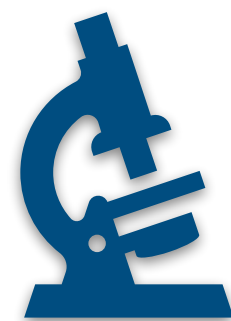
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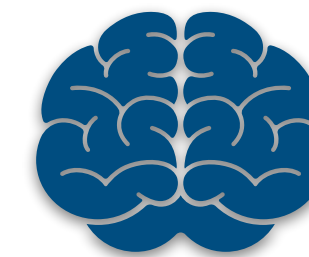
Example 2

*Training
quantum neural networks*

ρ : input state encoding classical input x

\mathcal{E} : the quantum neural network to learn

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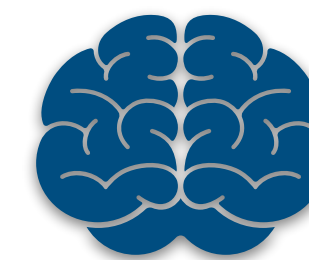
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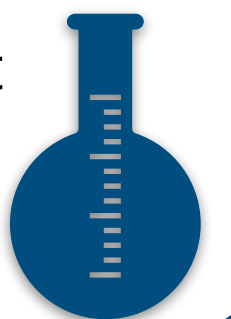
Example 3

*Speeding up
complex quantum dynamics*

ρ : initial state of the physical system

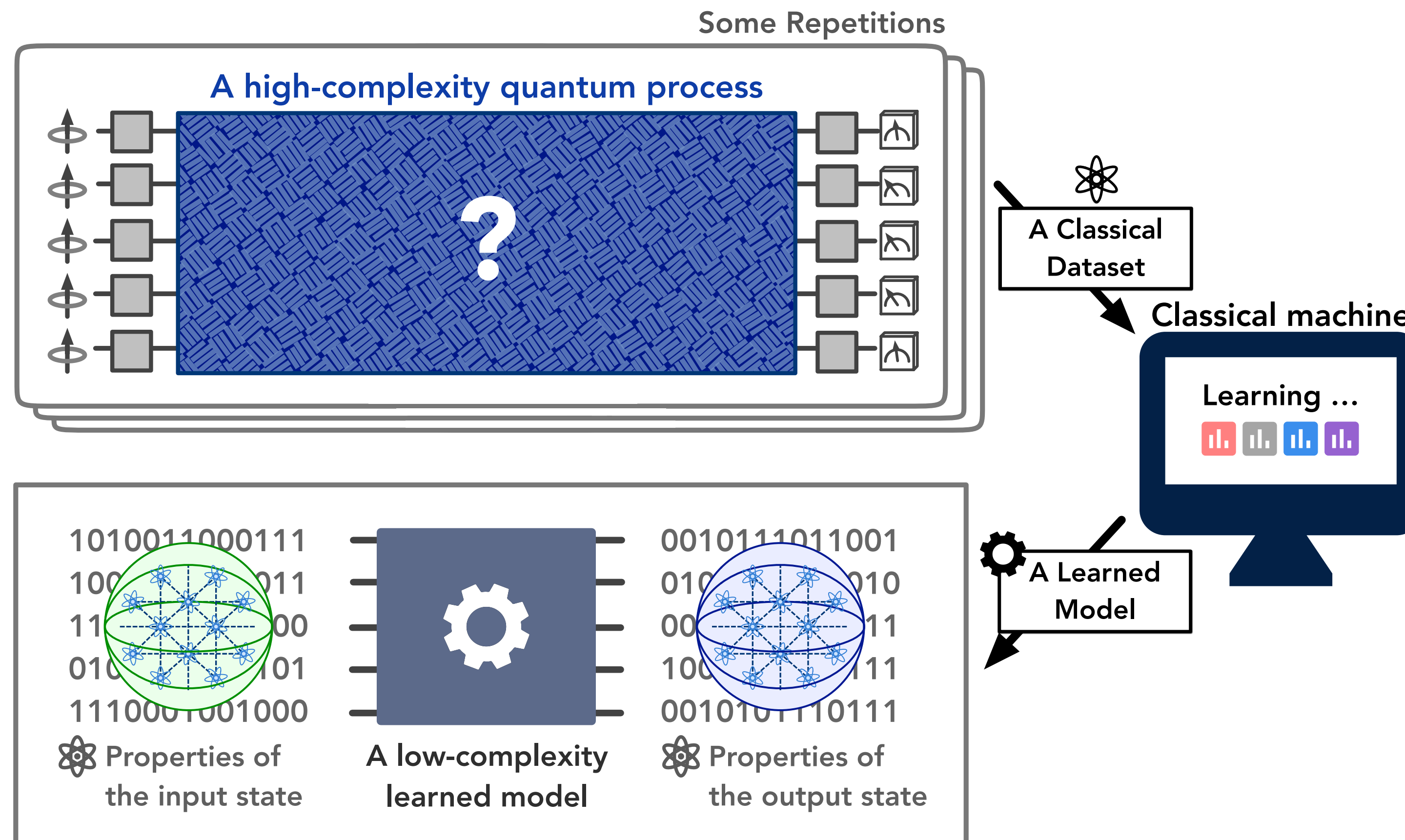
\mathcal{E} : the quantum dynamics to speed up

O : the property we want to predict



The goal of this work

Given an n -qubit CPTP map \mathcal{E} that represents a high-complexity quantum process



Overview

- A classical version of the quantum problem
- A restricted version of the quantum problem
- Generalization to the original quantum problem

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A Classical Problem

- Given an unknown classical Boolean circuit C mapping n bits to n bits.
- The input is now an n -bit string $x \in \{-1, 1\}^n$.
- The 1st output bit of C for input x is equal to $f_C(x) = \text{Tr}(Z_1 C(|x\rangle\langle x|))$.



Worst-case hardness

- The function f_C is equiv. to an exponentially long vector $\{-1,1\}^{2^n}$ with **no structure**.
- To learn a model $h(x)$, such that $|h(x) - f_C(x)|^2 < 0.5, \forall x \in \{-1,1\}^n$, we must query $f_C(x)$ for all input x . Query complexity: $\Theta(2^n)$.



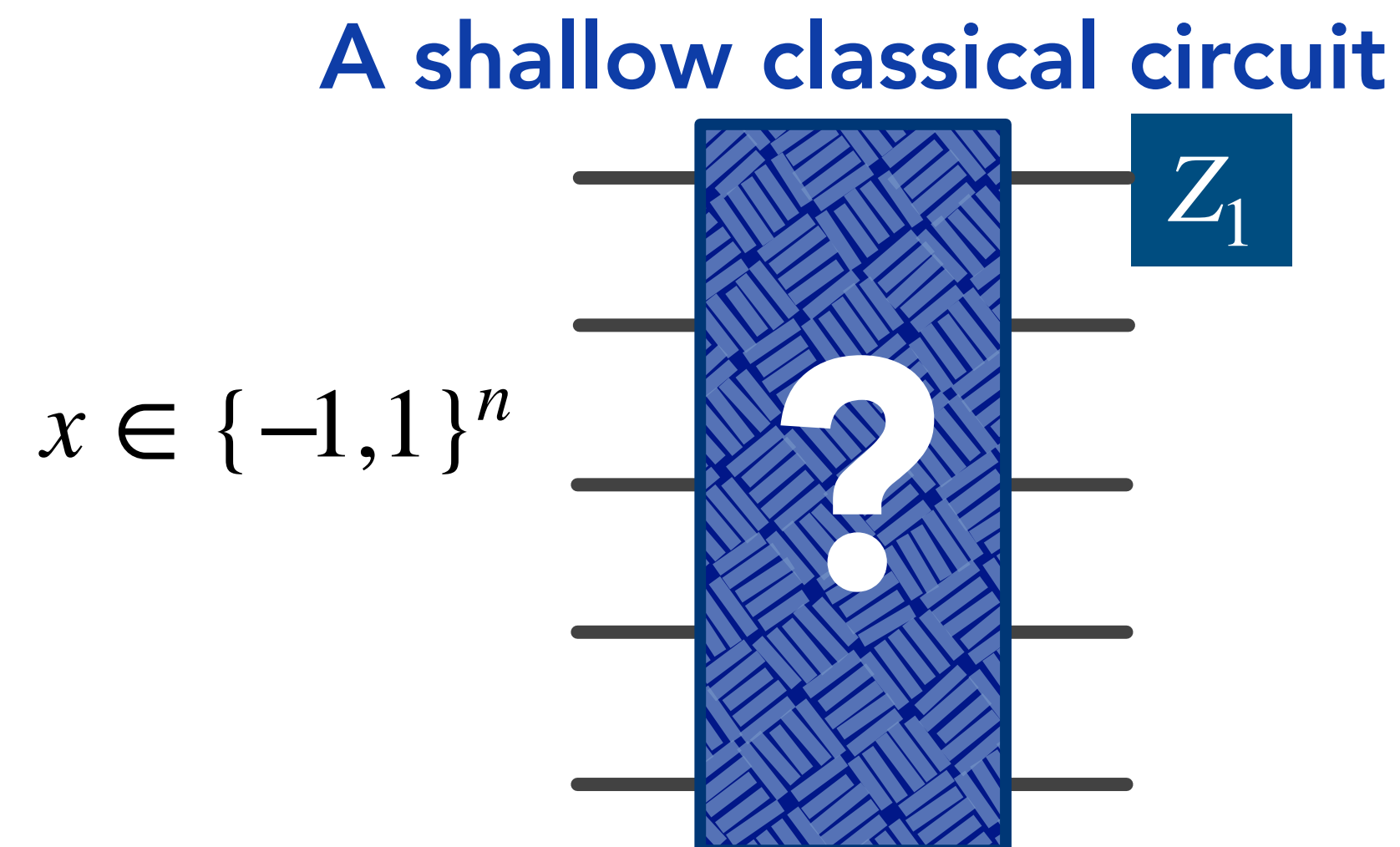
Average-case hardness

- The function f_C is equiv. to an exponentially long vector $\{-1,1\}^{2^n}$ with **no structure**.
- To learn a model $h(x)$, such that $\mathbb{E}_{x \sim \{-1,1\}^n} |h(x) - f_C(x)|^2 < 0.5$, we must query $f_C(x)$ for at least half of all x . Query complexity: $\Theta(2^n)$.



Average-case hardness for shallow classical circuits

- [AGS19] showed that learning $h(x)$, such that $\mathbb{E}_{x \sim \{-1,1\}^n} |h(x) - f_C(x)|^2 < 0.5$, is computationally hard (for both classical & quantum computers), even when the classical Boolean circuit is **constant-depth** (with majority gates, i.e., TC_0).



Overview

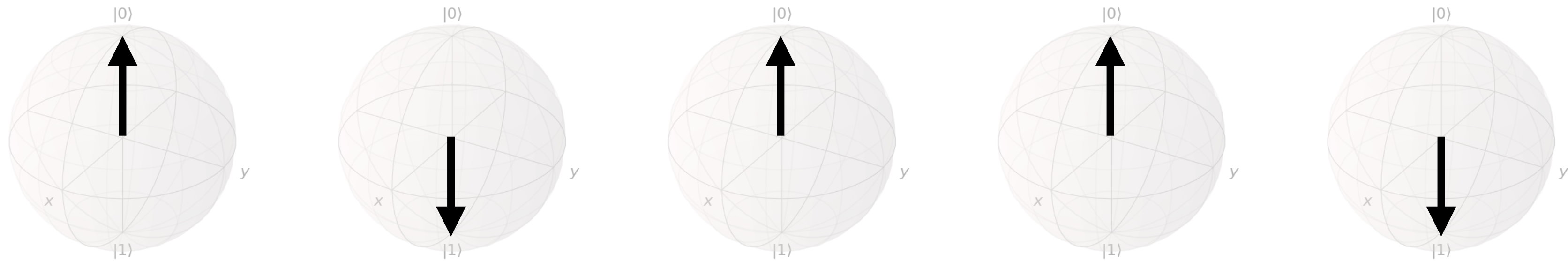
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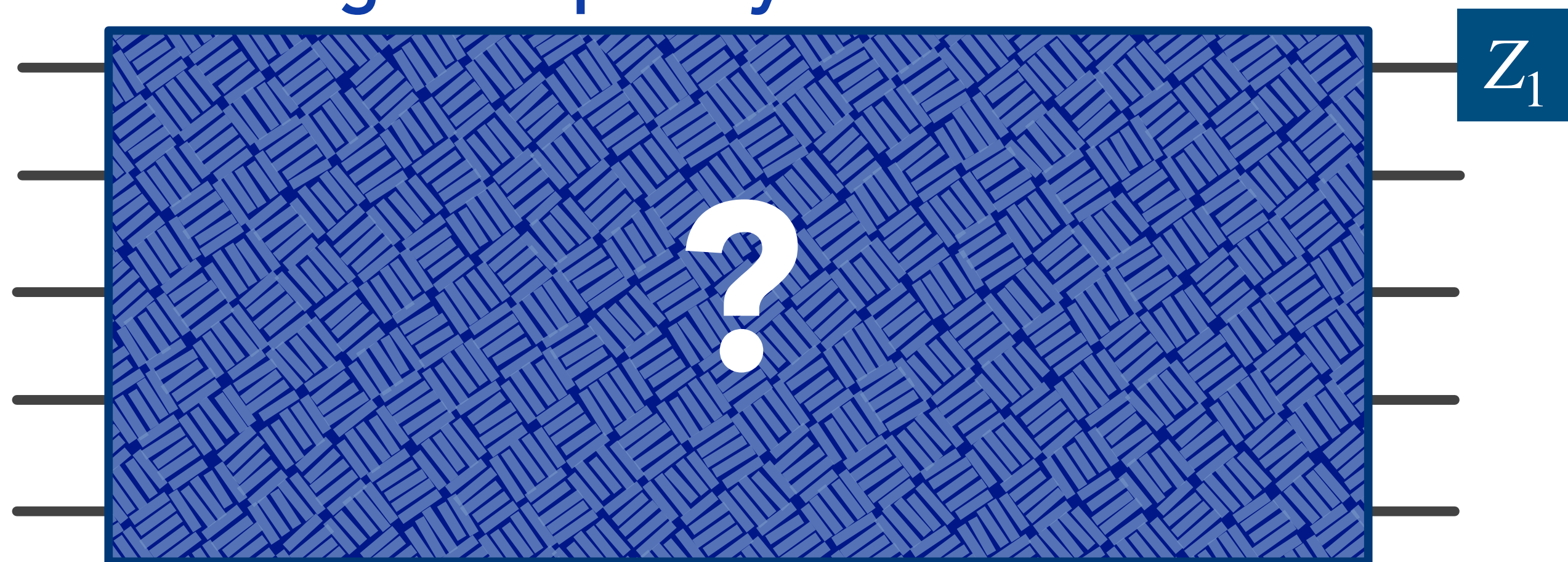
A Classical Problem

Input:



A high-complexity classical circuit

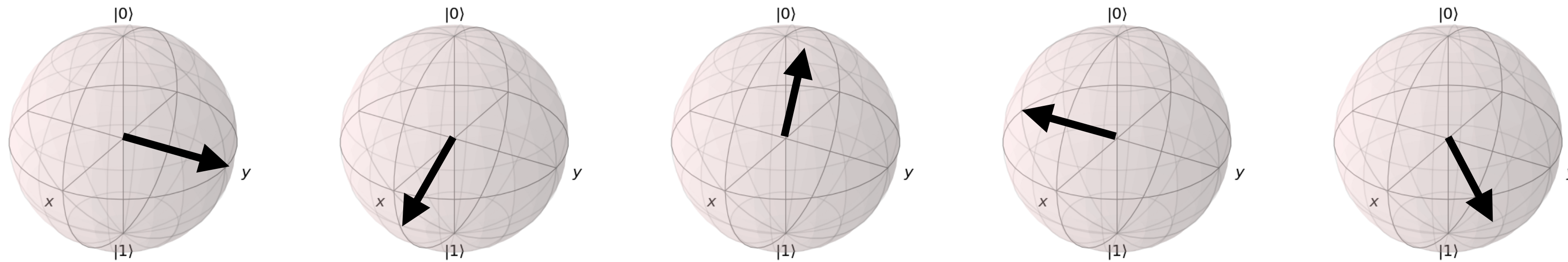
$$x \in \{-1, 1\}^n$$



This is hard!

A Quantum Problem

Input:



A high-complexity quantum process

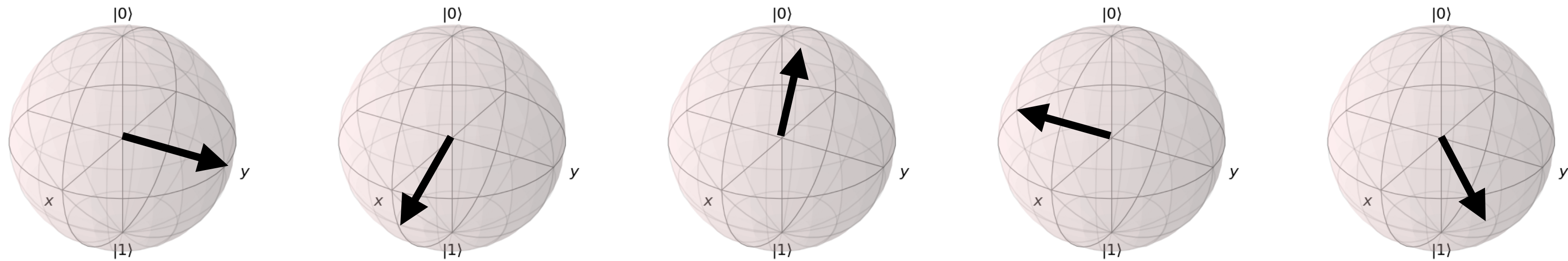
$$\bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$$



Is this harder?

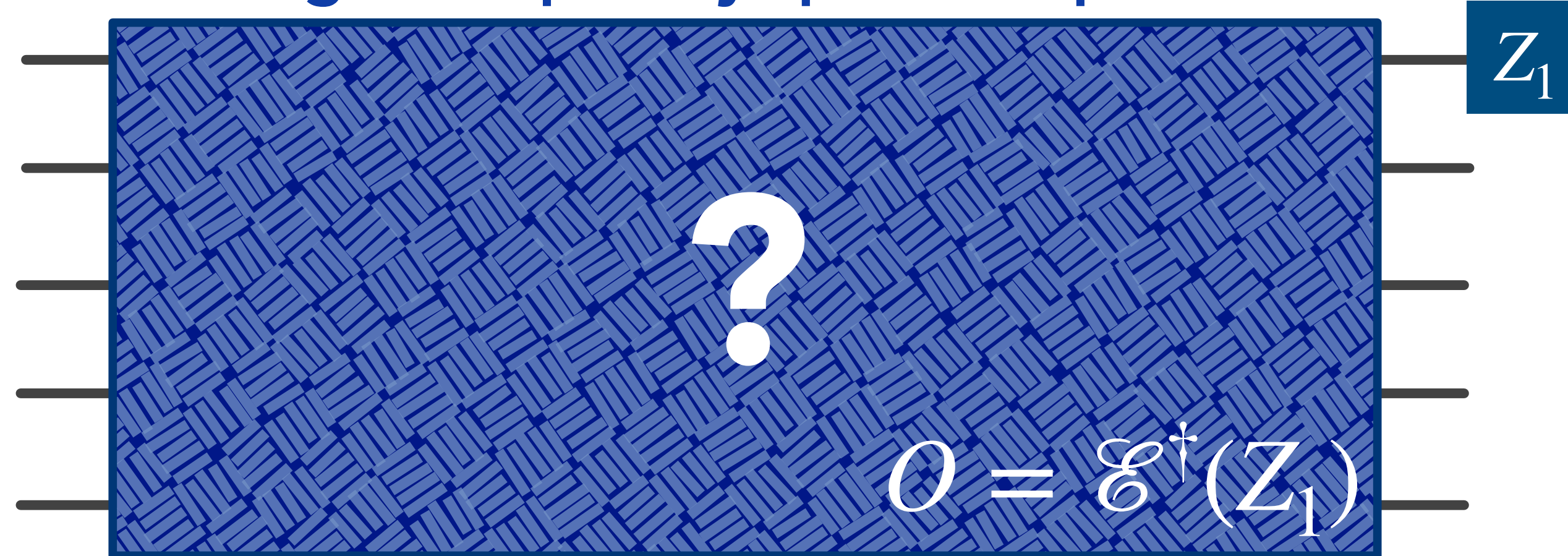
A Quantum Problem

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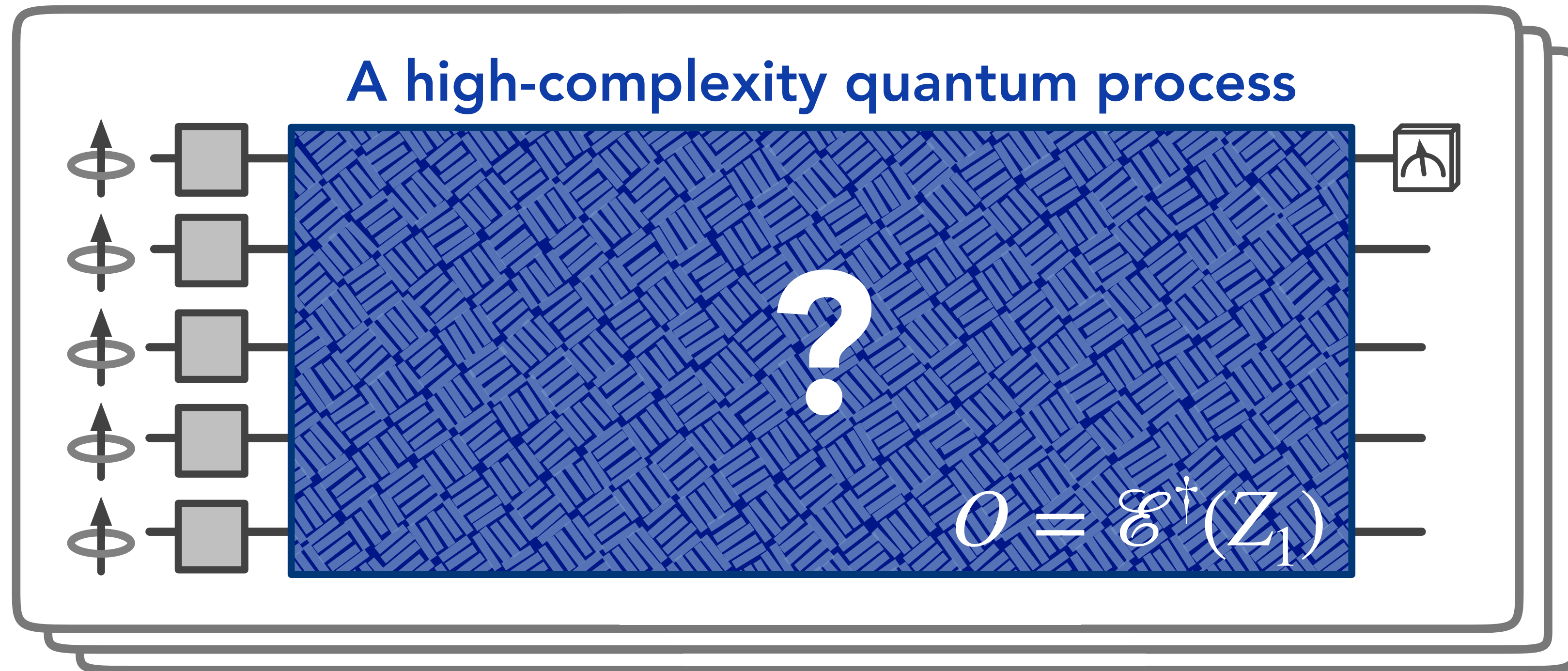
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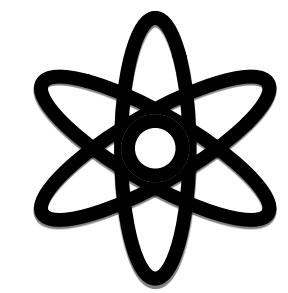
A Classical Dataset

Some Repetitions



Each repetition prepares a random product state, and measures the 1st qubit in the Z basis

A Classical Dataset



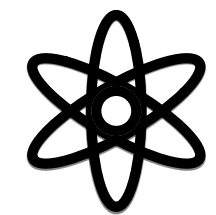
Classical Dataset about O

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

for $\ell = 1, \dots, N$.

Each repetition prepares a random product state, and measures the 1st qubit in the Z basis

The Prediction Task



Classical Dataset about O

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

for $\ell = 1, \dots, N$.

Given a new state $|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$,

how to predict $\langle \psi | O | \psi \rangle$ accurately?

Worst-case hardness

- To learn a model $h(|\psi\rangle)$, such that $\left| h(|\psi\rangle) - \langle \psi | O | \psi \rangle \right|^2 < 0.5, \forall |\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle$, the problem is at least as hard as the classical problem.
- Hence, the query complexity is $\Omega(2^n)$.



Average-case hardness?

- To learn a model $h(|\psi\rangle)$, such that $\mathbb{E}_{|\psi\rangle=\bigotimes_{i=1}^n |\psi_i\rangle} \left| h(|\psi\rangle) - \langle \psi | O | \psi \rangle \right|^2 < 0.5$, is the problem still exponentially hard?
- Surprisingly, the answer is **no**. The problem can be done in quasi-polynomial time.



Low-weight approximation

$$O = \sum_{P \in \{I, X, Y, Z\}^{\otimes n}} \alpha_P P$$

$$O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$$

Lemma (Low-weight approximation): $\mathbb{E}_{|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle} \left| \langle \psi | O | \psi \rangle - \langle \psi | O^{(\text{low})} | \psi \rangle \right|^2 < \frac{1}{3^k}$.

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Interpretation: For most product state $|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle$, $\langle \psi | O | \psi \rangle \approx \langle \psi | O^{(\text{low})} | \psi \rangle$.

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Interpretation: For most product state $|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle$, $\langle \psi | O | \psi \rangle \approx \langle \psi | O^{(\text{low})} | \psi \rangle$.

Low-weight approximation **does not** hold in the classical version of this problem

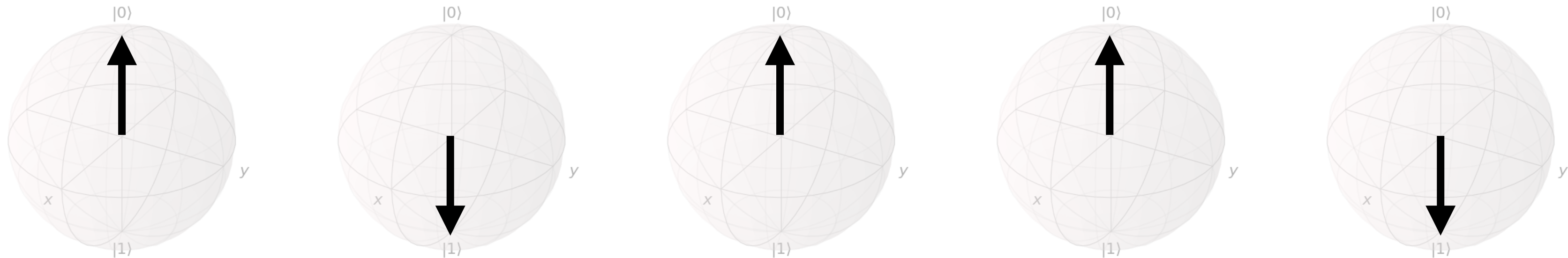
Low-weight approximation

$$O = \sum_{P \in \{I, X, Y, Z\}^{\otimes n}} \alpha_P P$$

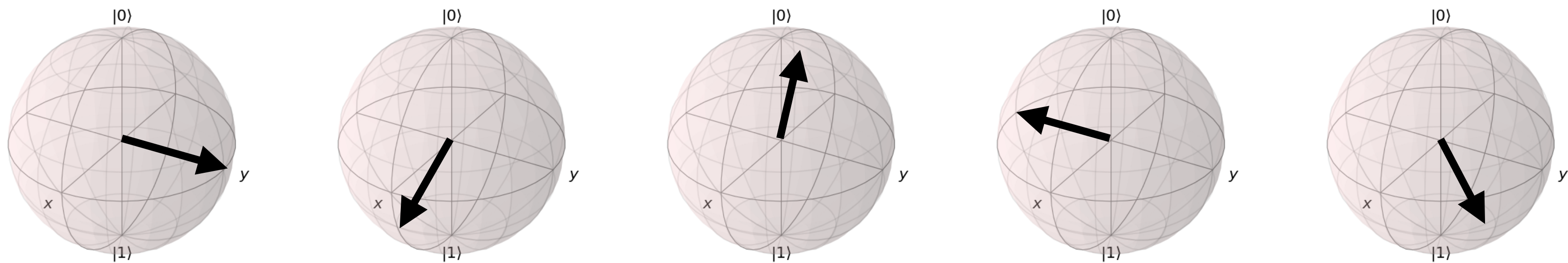
$$O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$$

Classical inputs are perfectly distinguishable.
But quantum state inputs are not.

Classical Input:



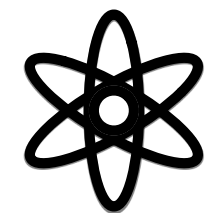
Quantum Input:



Basic Idea for the ML model

Basic idea: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Lemma (Fourier transform): $\alpha_P = \mathbb{E} \left[\frac{3^{|P|}}{N} \sum_{\ell=1}^N y_\ell \langle \psi_\ell | P | \psi_\ell \rangle \right], \forall P \in \{I, X, Y, Z\}^{\otimes n}$



Classical Dataset

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for $\ell = 1, \dots, N$.

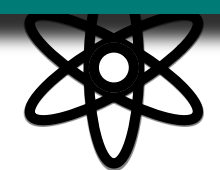
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Lemma

How large should the data size N be?

$\{X, Z\}^{\otimes n}$



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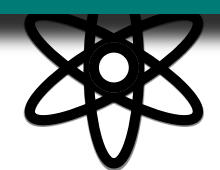
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Lemma

We only need $N = \mathcal{O}(\log n)$!

$\{X, Z\}^{\otimes n}$



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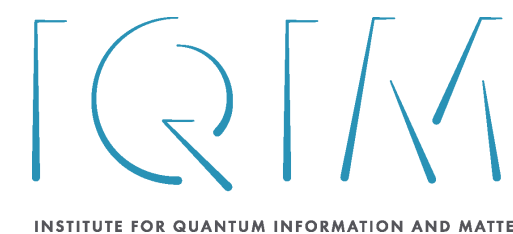
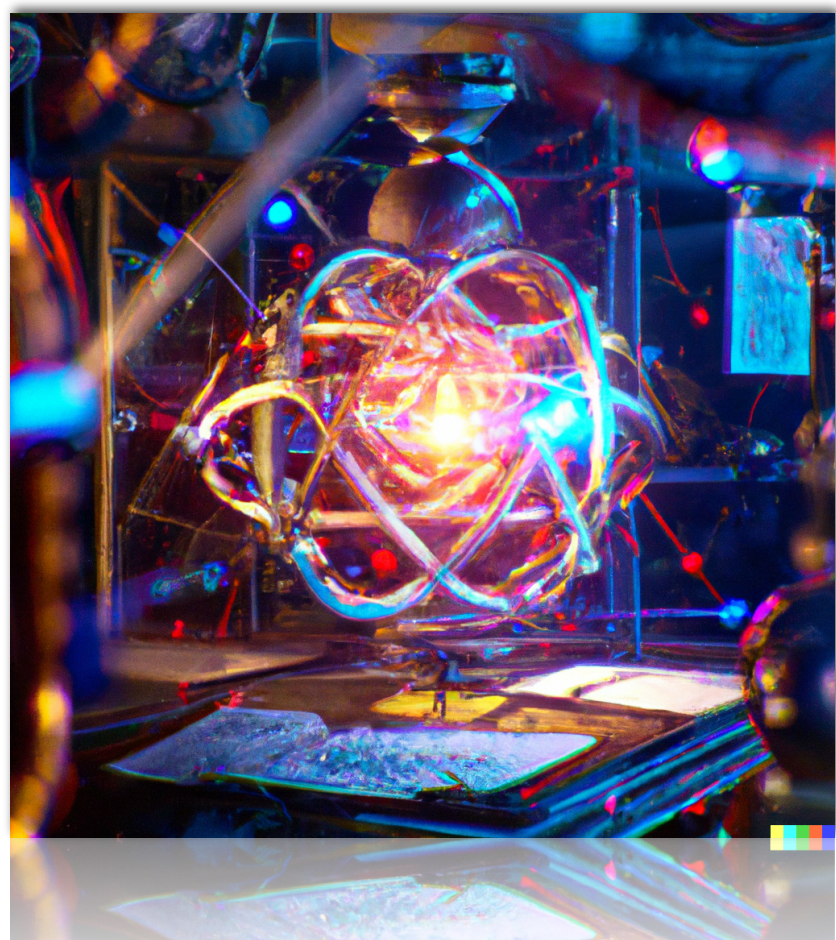
for $\ell = 1, \dots, N$.

An interlude

Optimizing Quantum Hamiltonians

Presenter: Hsin-Yuan Huang (Robert)

Joint work with Sitan Chen and John Preskill



The Task

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

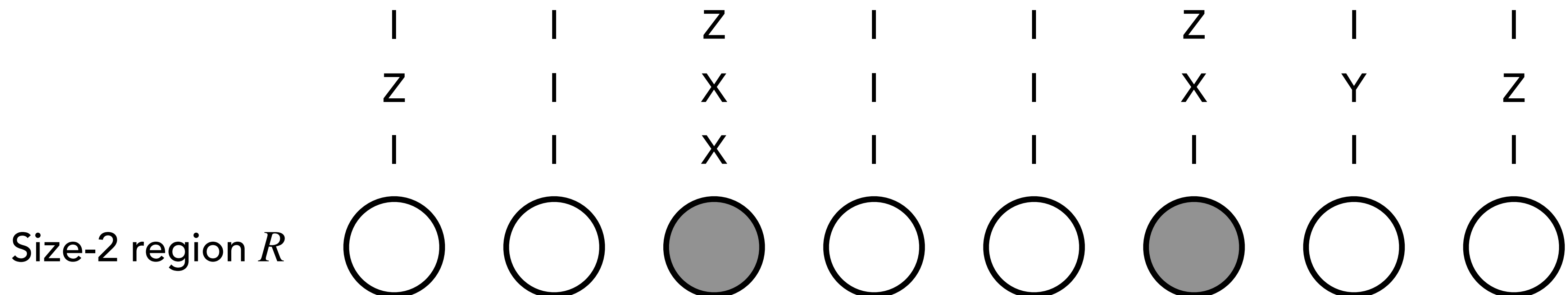
Find a state $|\psi\rangle$ that maximizes or minimizes $\langle \psi | H | \psi \rangle$.

We want a guarantee on $\langle \psi | H | \psi \rangle$
based on the description of $H = \sum_{|P| \leq k} \alpha_P P$

Expansion property

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

H has an expansion coefficient c_e and dimension d_e if for every size- d_e region R , the number of P with $\alpha_P \neq 0$, $\text{dom}(P) \subseteq R$, $R \subseteq \text{dom}(P)$ is at most c_e .



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Example 1

Geometrically-local Hamiltonian

$$c_e = \mathcal{O}(1), d_e = 1$$

Example 2

General k -local Hamiltonian

$$c_e = 4^k, d_e = k$$

Example 3

Degree- d 2-body Hamiltonian

$$c_e = 16d, d_e = 1$$

Theorem

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

If H has an expansion coefficient c_e and dimension d_e , then for $r = 2d_e/(d_e + 1) \in [1, 2)$, we have an algorithm that either finds a maximizing product state $|\psi\rangle$,

$$\langle \psi | H | \psi \rangle \geq \mathbb{E}_{|\phi\rangle: \text{Haar}} \langle \phi | H | \phi \rangle + \frac{1}{c_e^{1/2d_e} 2^{\Theta(k \log k)}} \left(\sum_{P \neq I} |\alpha_P|^r \right)^{1/r},$$

or finds a minimizing product state $|\psi\rangle$ with a similar guarantee ($+ \rightarrow -$, $\geq \rightarrow \leq$).

Theorem

Improved over existing results

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The Algorithm

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

Find a product state $|\psi\rangle$ that approximately optimizes $\langle \psi | H | \psi \rangle$.

The Algorithm

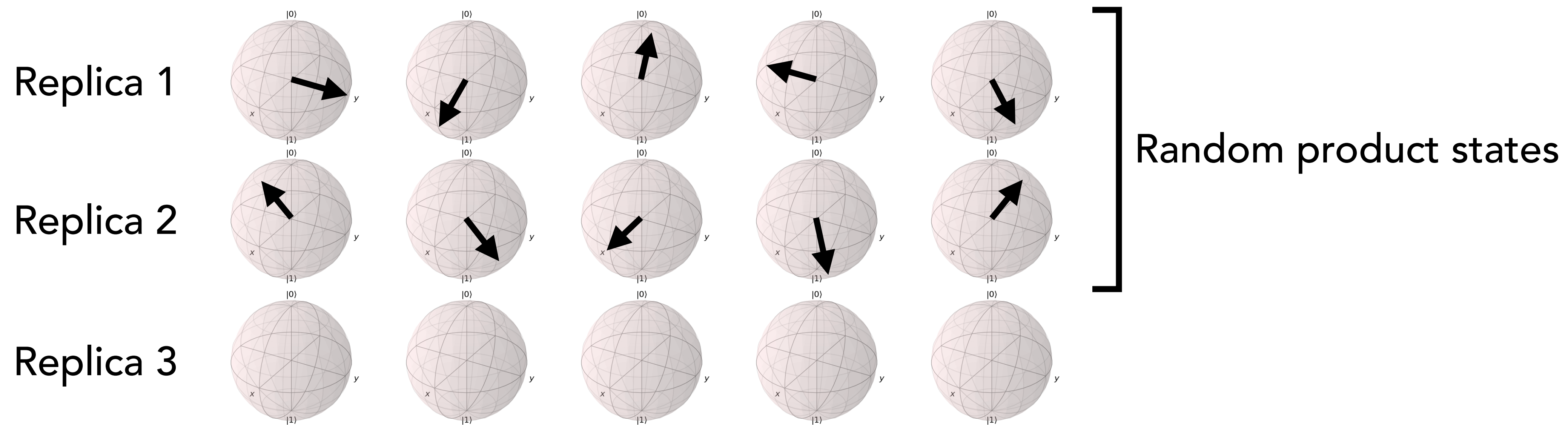
Select a slice with the largest value of α_P

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.

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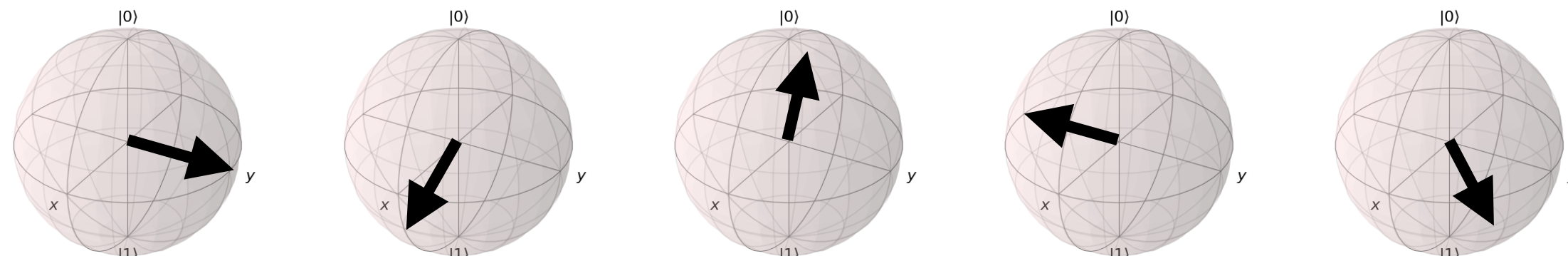


The Algorithm

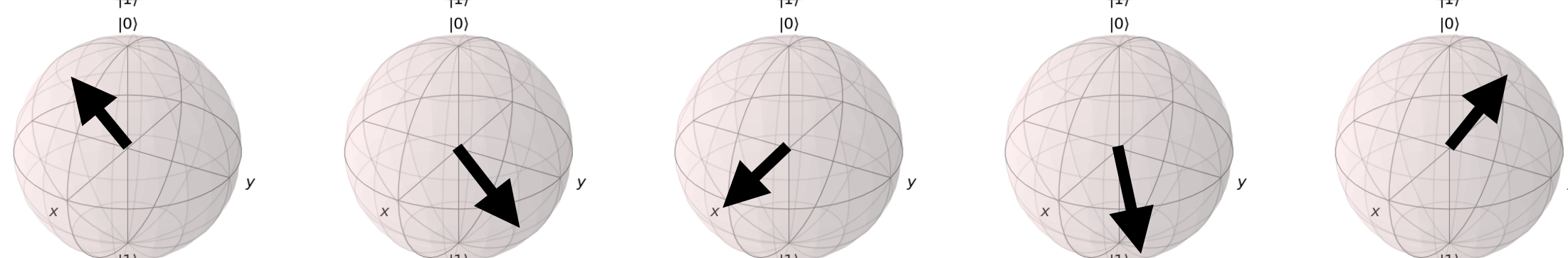
Lift n -qubit H to nk qubits

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.

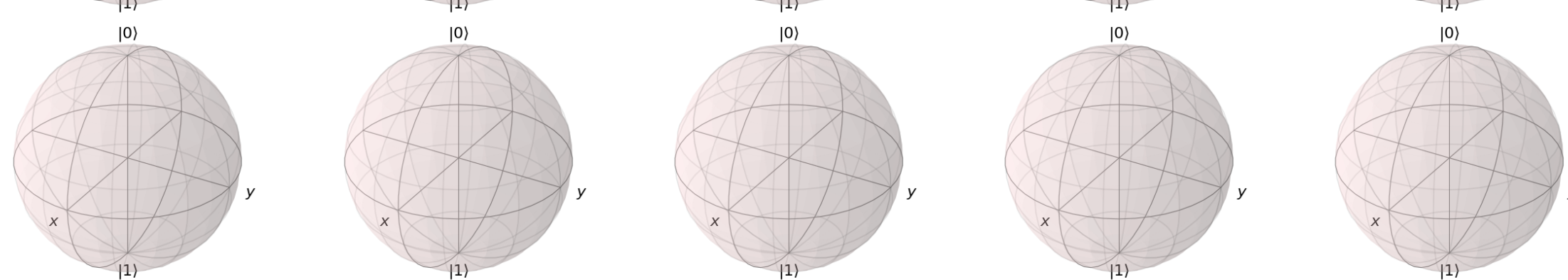
Replica 1



Replica 2



Replica 3

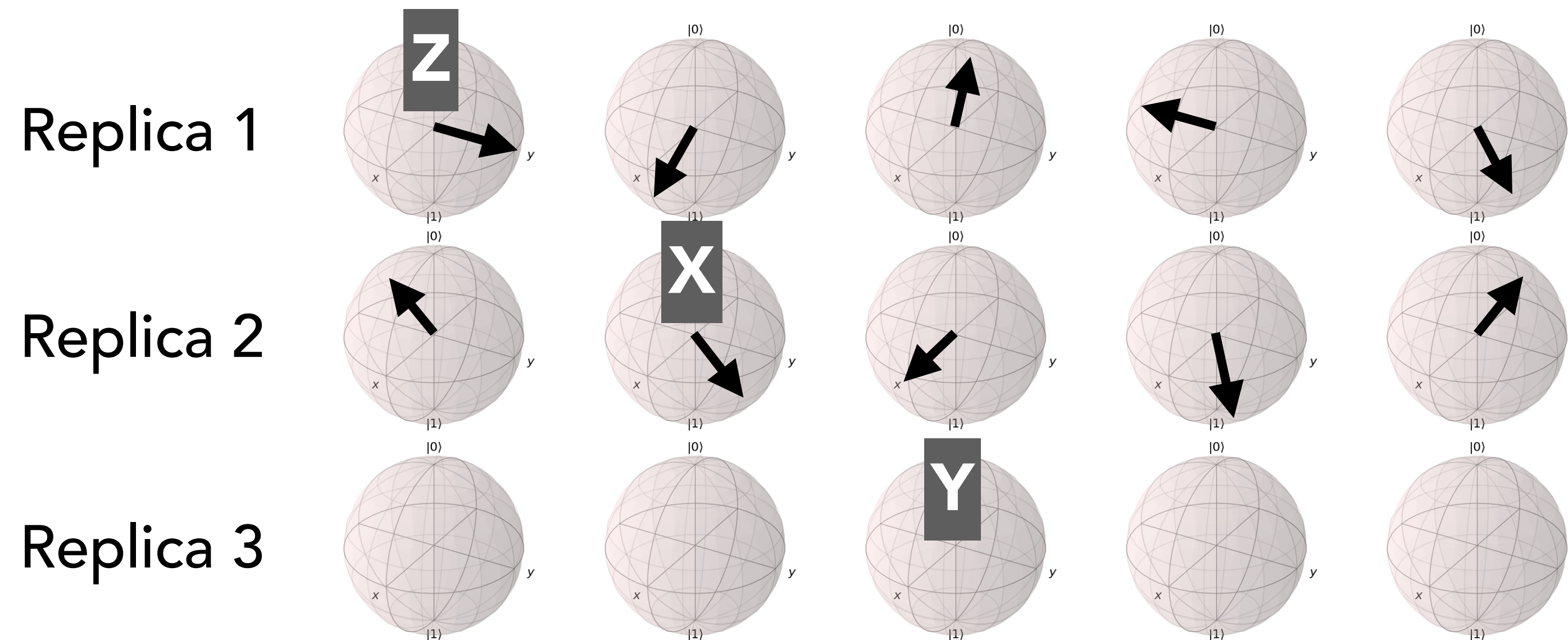


$$\text{pol}(H) = \sum_{|P|=k} \alpha_P \text{pol}(P) \in \mathbb{C}^{2^{nk} \times 2^{nk}}$$

The Algorithm

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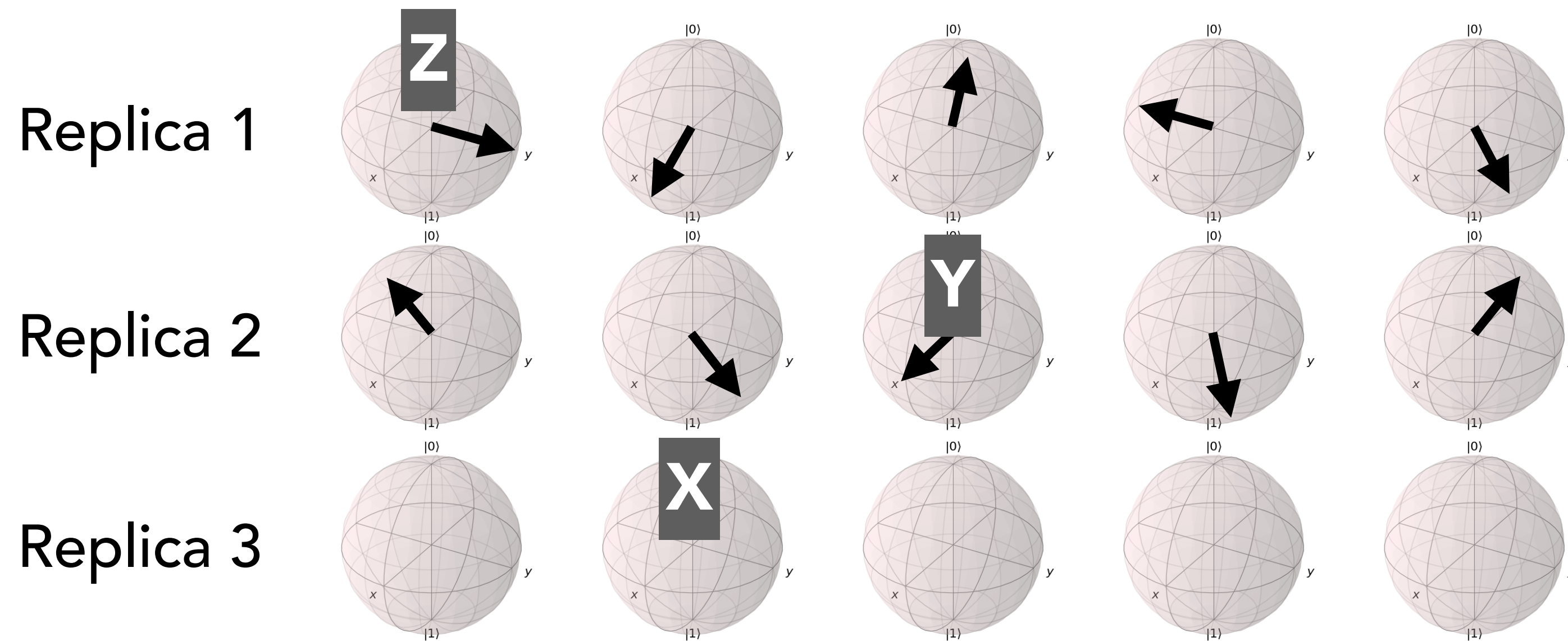
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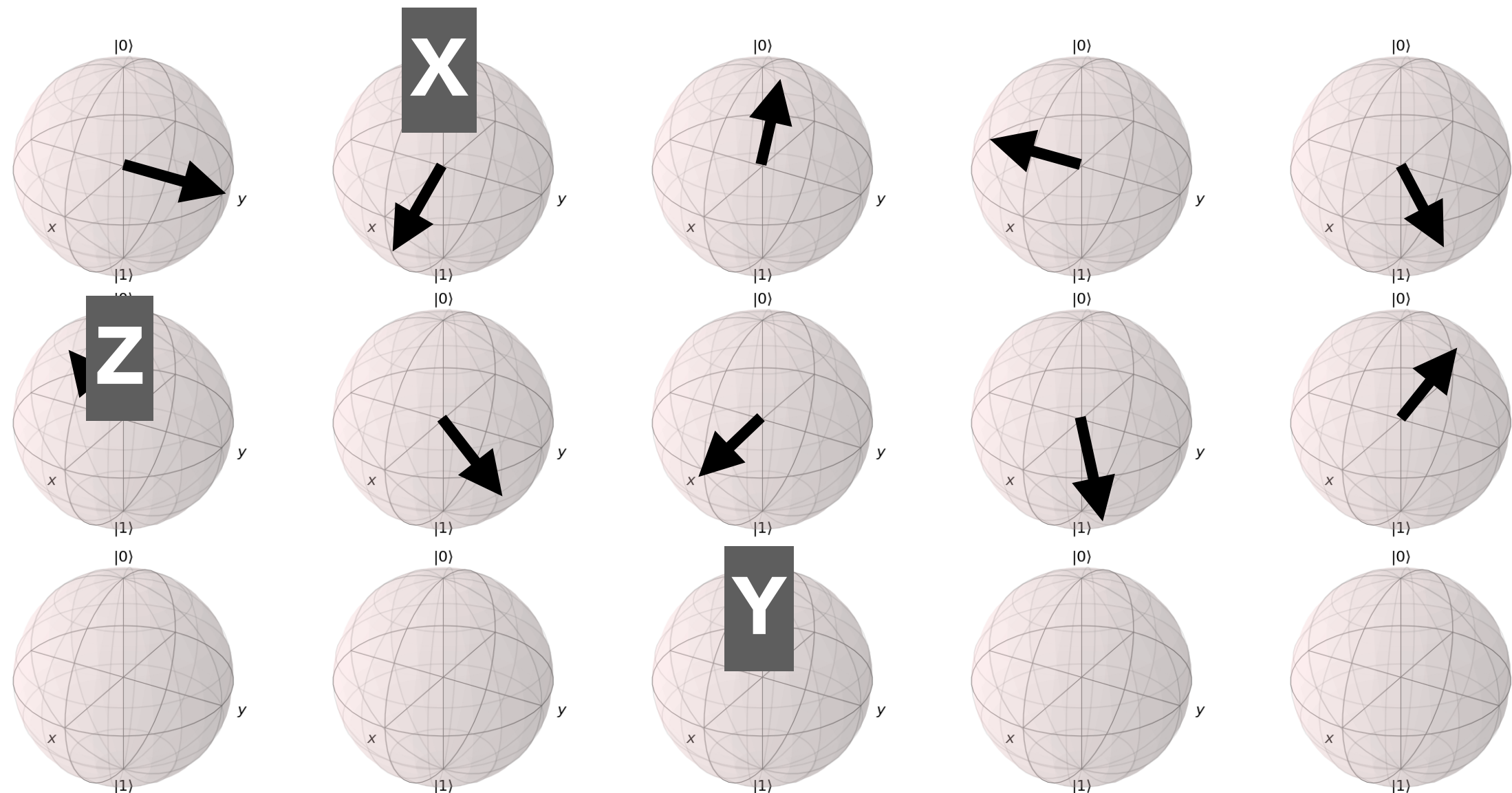
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Replica 2

Replica 3

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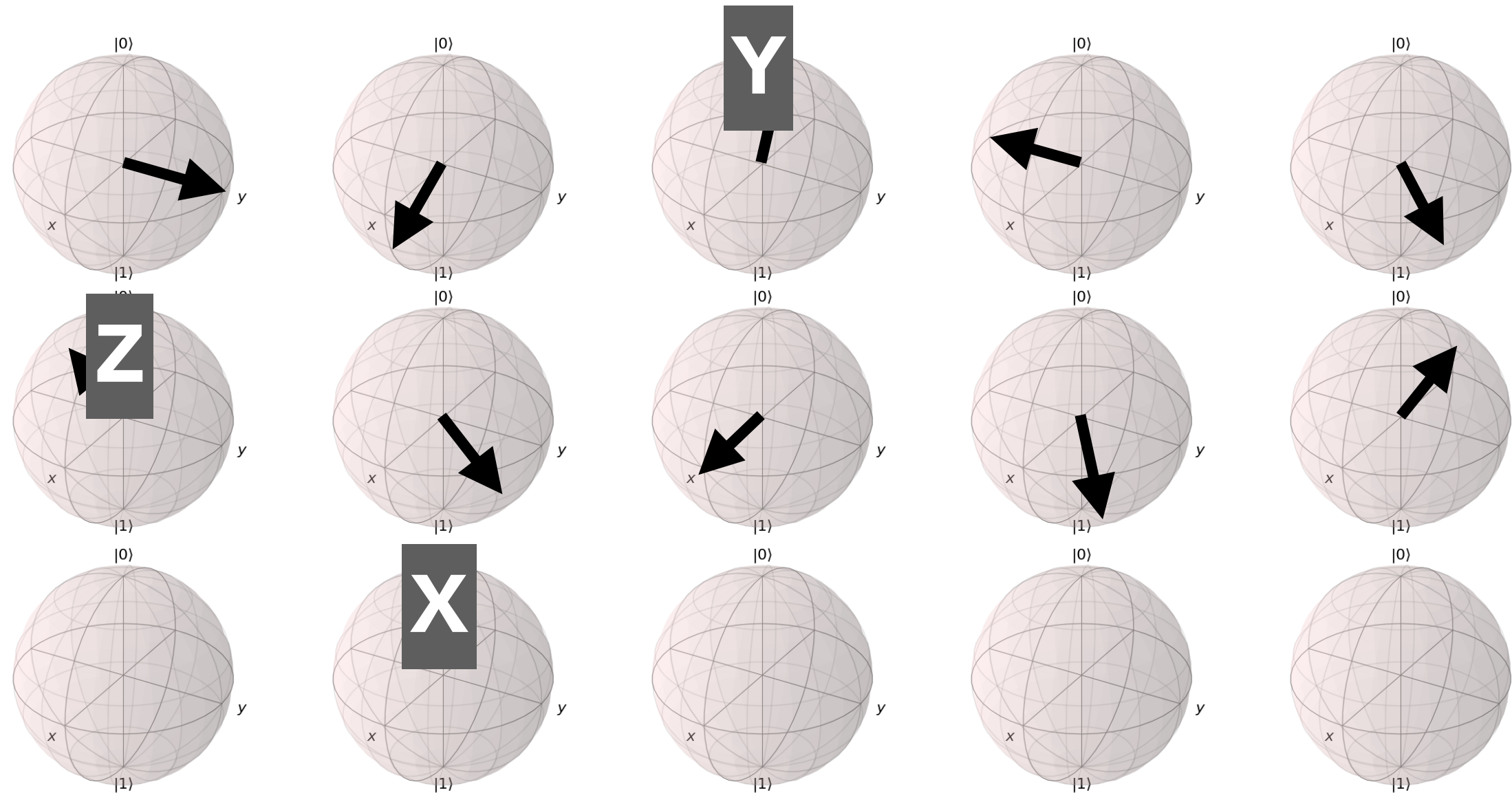
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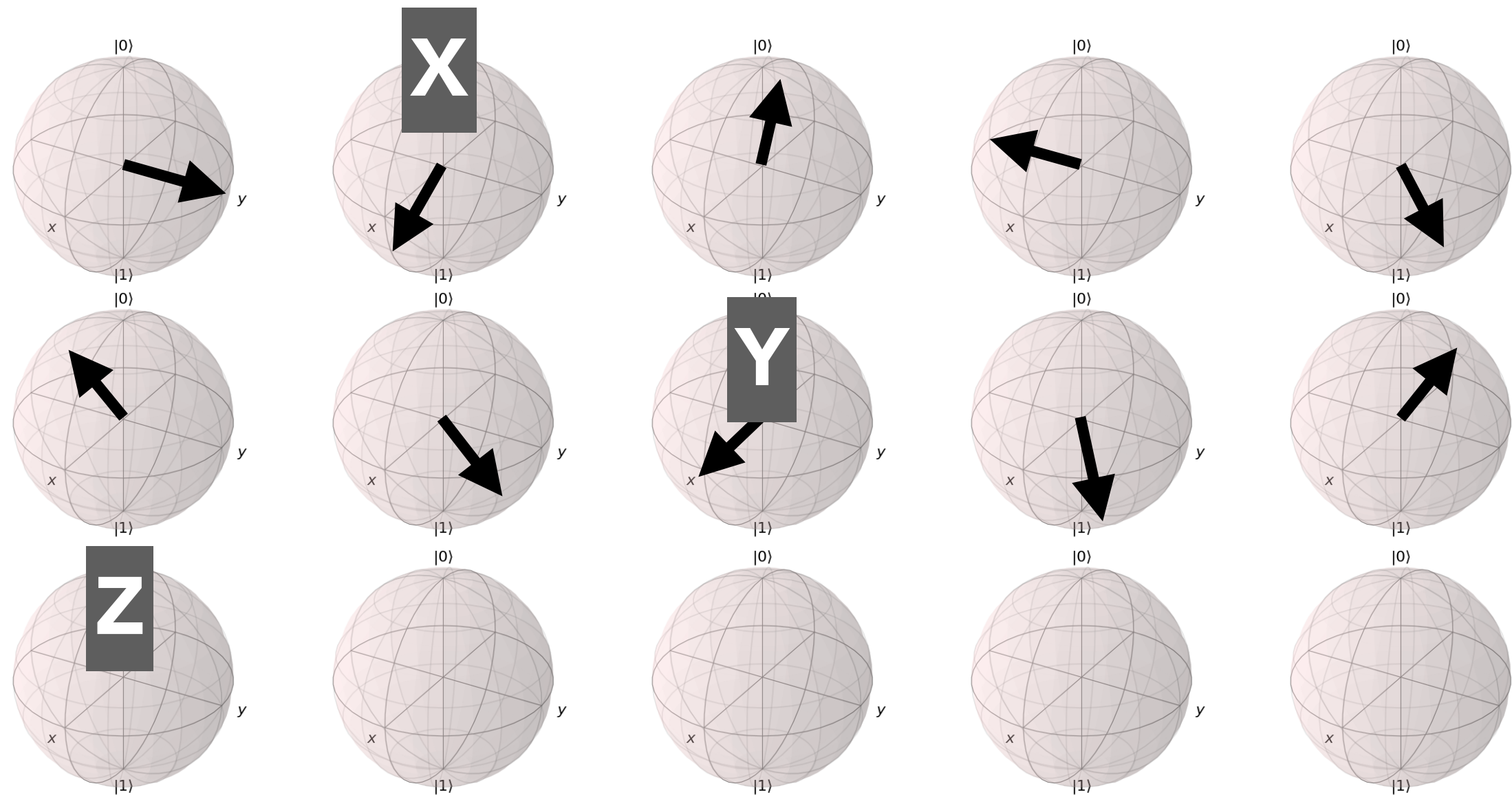
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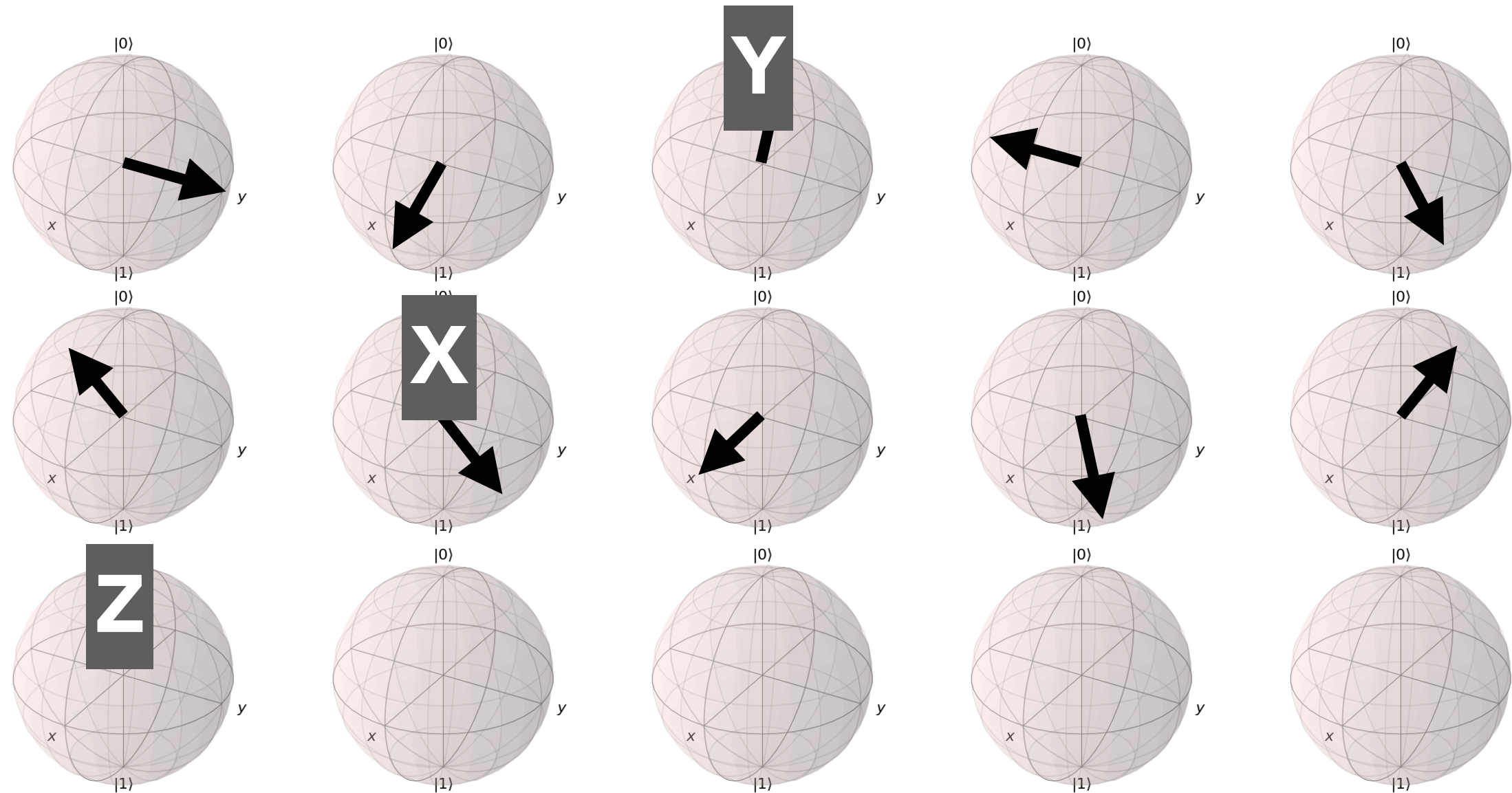
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Replica 2

Replica 3

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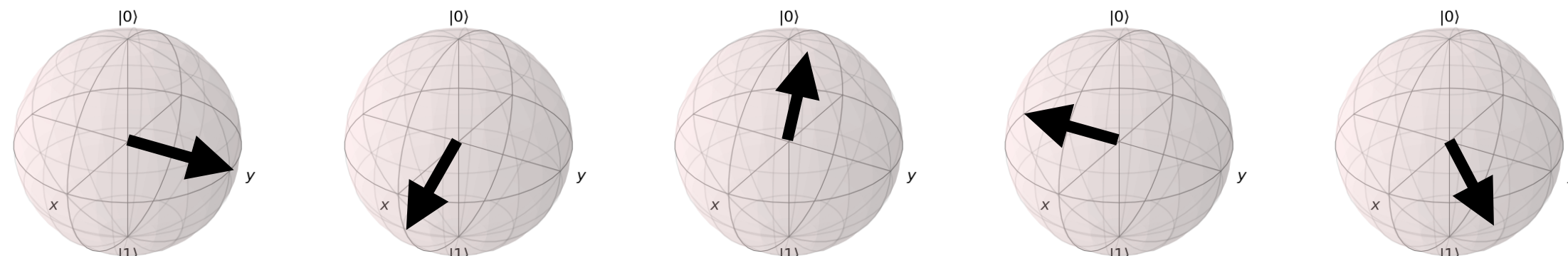
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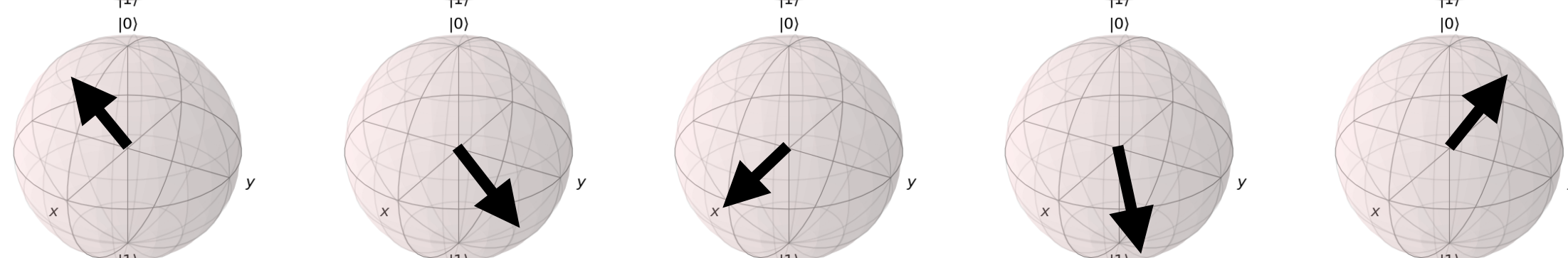
Lift n -qubit H to nk qubits

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.

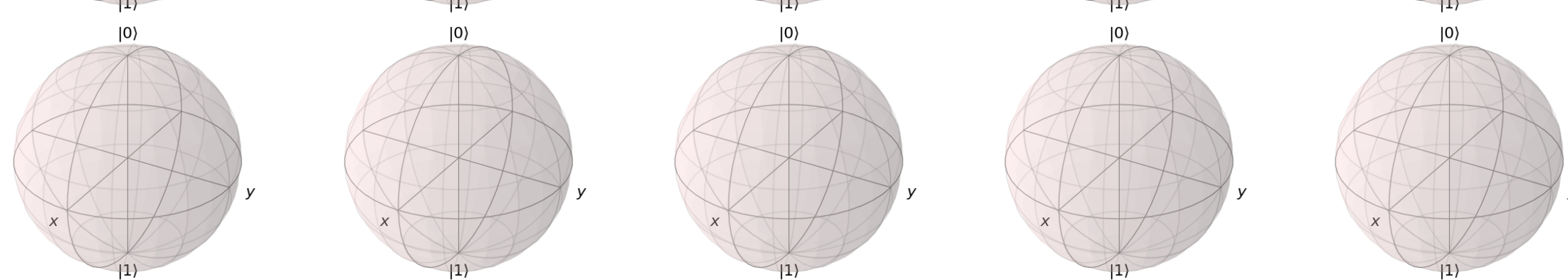
Replica 1



Replica 2



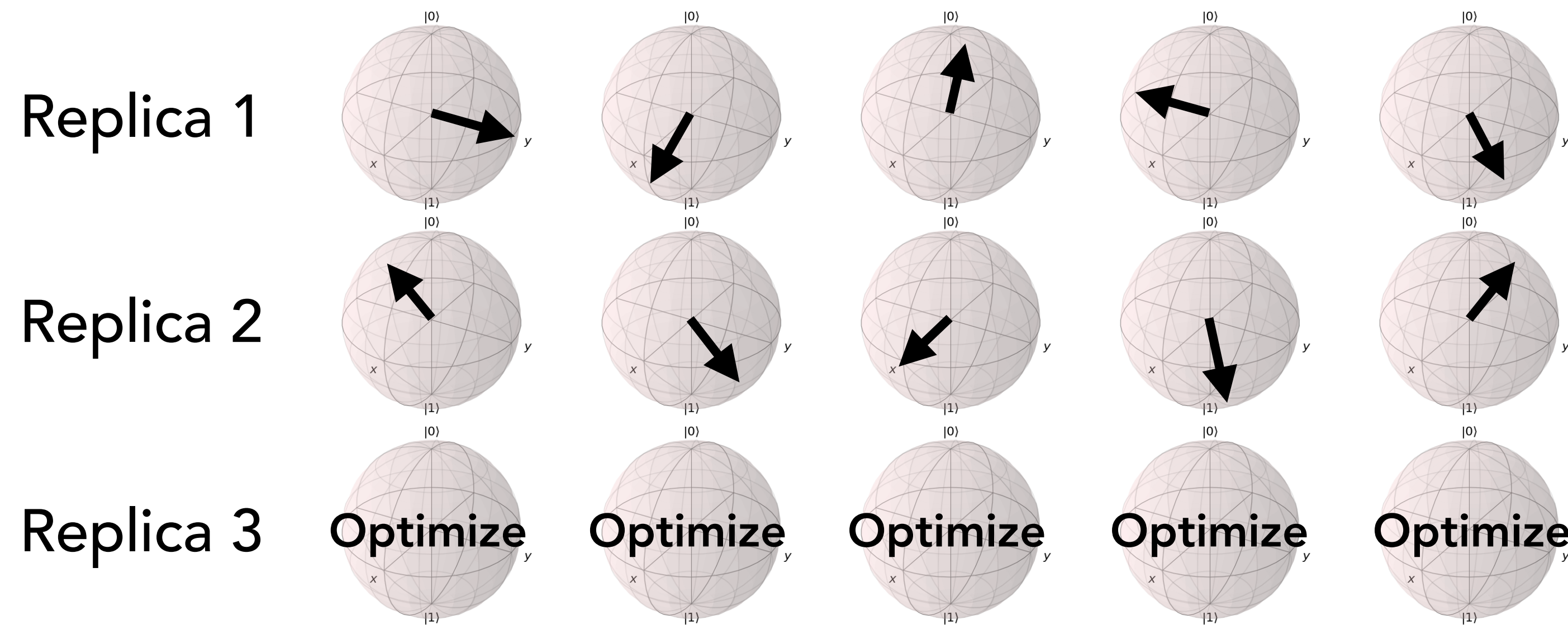
Replica 3



$$\text{pol}(H) = \sum_{|P|=k} \alpha_P \text{pol}(P) \in \mathbb{C}^{2^{nk} \times 2^{nk}}$$

The Algorithm

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.

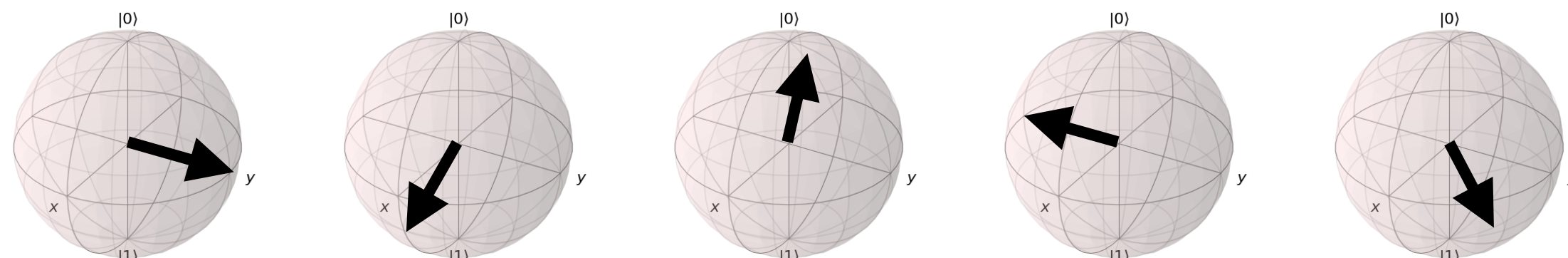


$$\text{pol}(H) = \sum_{|P|=k} \alpha_P \text{pol}(P) \in \mathbb{C}^{2^{nk} \times 2^{nk}}$$

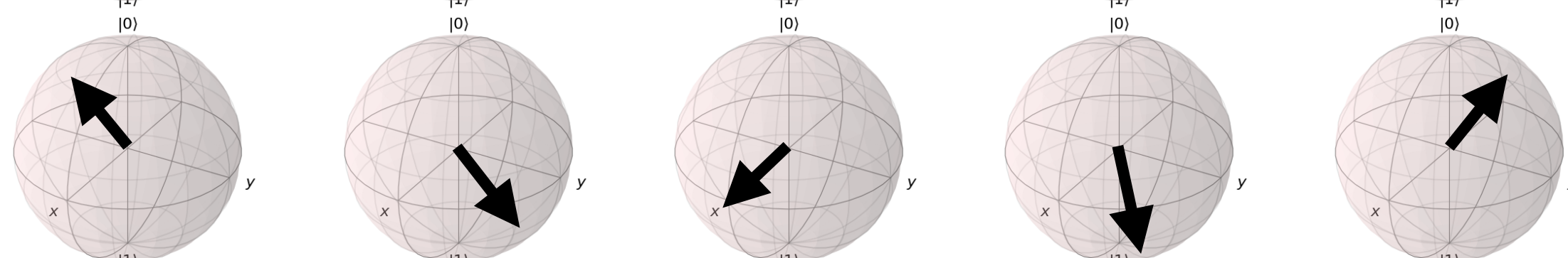
The Algorithm

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.

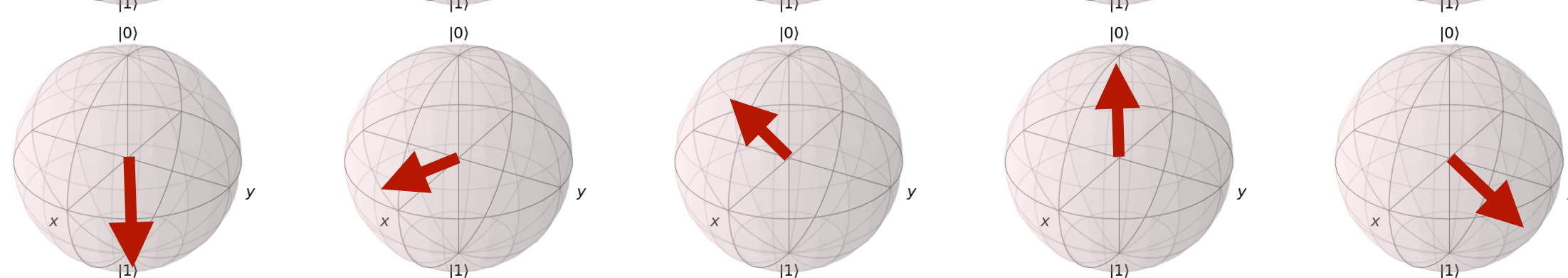
Replica 1



Replica 2



Replica 3

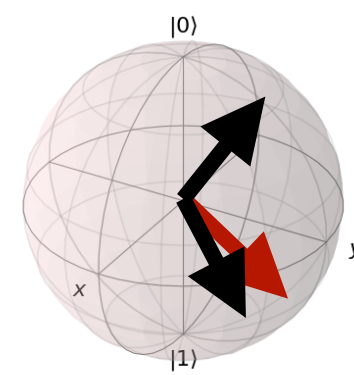
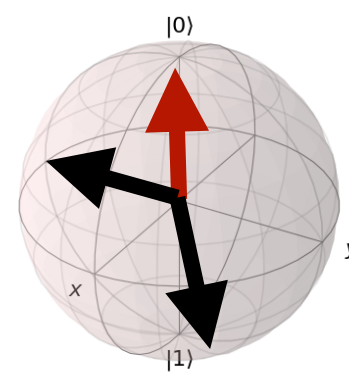
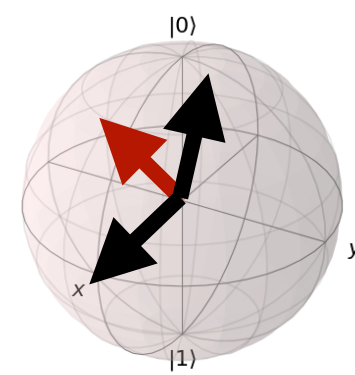
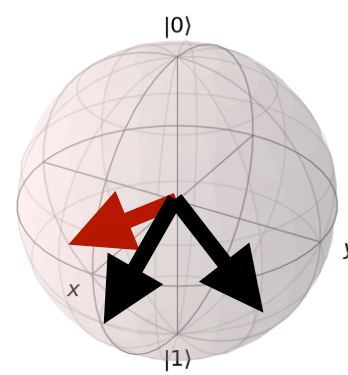
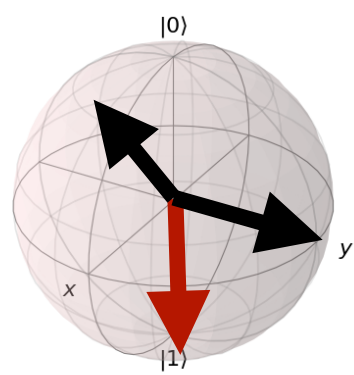


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The Algorithm

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.

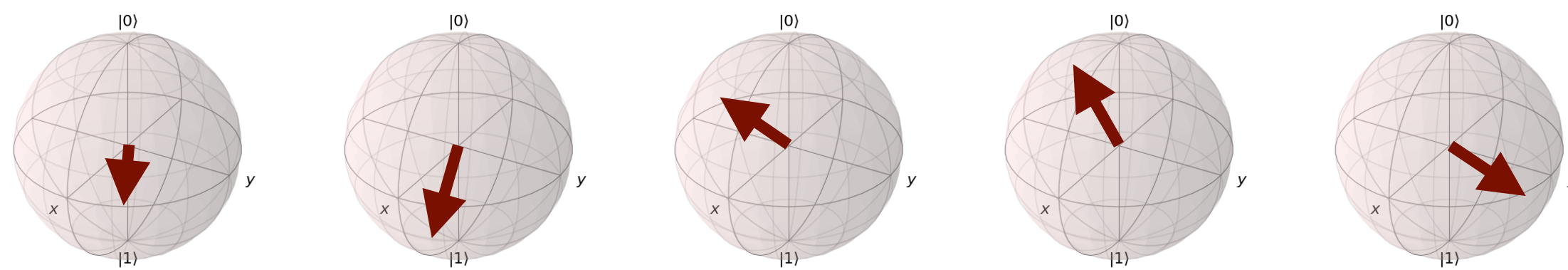
Replica



Combine the Bloch vectors using a weighted sum

The Algorithm

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.



Combine the Bloch vectors
using a weighted sum

Theorem

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

If H has an expansion coefficient c_e and dimension d_e , then for $r = 2d_e/(d_e + 1) \in [1, 2)$, we have an algorithm that either finds a maximizing product state $|\psi\rangle$,

$$\langle \psi | H | \psi \rangle \geq \mathbb{E}_{|\phi\rangle: \text{Haar}} \langle \phi | H | \phi \rangle + \frac{1}{c_e^{1/2d_e} 2^{\Theta(k \log k)}} \left(\sum_{P \neq I} |\alpha_P|^r \right)^{1/r},$$

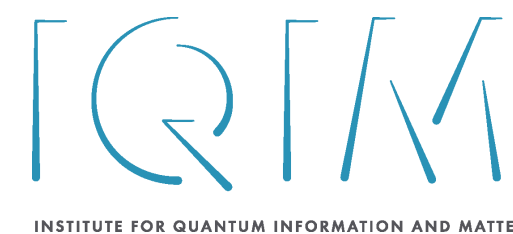
or finds a minimizing product state $|\psi\rangle$ with a similar guarantee ($+ \rightarrow -$, $\geq \rightarrow \leq$).

Another interlude

Generalized Quantum Bohnenblust-Hille Inequality

Presenter: Hsin-Yuan Huang (Robert)

Joint work with Sitan Chen and John Preskill



Theorem

Given an observable $O = \sum_{|P| \leq k} \alpha_P P$ with an expansion coefficient c_e and dimension d_e .

$$\|O\|_{\infty} \geq \frac{1}{c_e^{1/2d_e} 2^{\Theta(k \log k)}} \left(\sum_P |\alpha_P|^r \right)^{1/r} \text{ for } r = \frac{2d_e}{d_e + 1} \in [1, 2).$$

Proof ideas:

- (1) Use the guarantee from the algorithm for optimizing quantum Hamiltonians.
- (2) Adapt by noting that $\|O\|_{\infty} \geq |\langle \psi | O | \psi \rangle|$, where $|\psi\rangle$ is the state found by the algo.

Theorem

Given an observable $O = \sum_{|P| \leq k} \alpha_P P$ with an expansion coefficient c_e and dimension d_e .

$$\|O\|_\infty \geq \frac{1}{c_e^{1/2d_e} 2^{\Theta(k \log k)}} \left(\sum_P |\alpha_P|^r \right)^{1/r} \text{ for } r = \frac{2d_e}{d_e + 1} \in [1, 2).$$

Example 1

A sum of geometrically-local terms

$$c_e = \mathcal{O}(1), d_e = 1$$

$$\sum_P |\alpha_P| \leq \mathcal{O}(\|O\|_\infty)$$

Theorem

Given an observable $O = \sum_{|P| \leq k} \alpha_P P$ with an expansion coefficient c_e and dimension d_e .

$$\|O\|_{\infty} \geq \frac{1}{c_e^{1/2d_e} 2^{\Theta(k \log k)}} \left(\sum_P |\alpha_P|^r \right)^{1/r} \text{ for } r = \frac{2d_e}{d_e + 1} \in [1, 2).$$

Example 2

A sum of k -local terms

$$c_e = 4^k, d_e = k$$

$$\|\vec{\alpha}\|_{\frac{2k}{k+1}} \leq 2^{\Theta(k \log k)} \|O\|_{\infty}$$

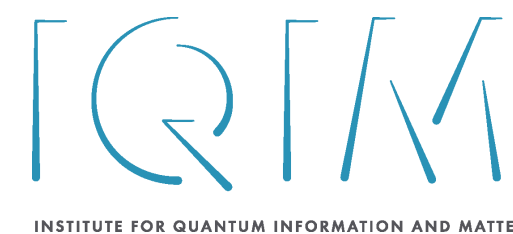
A quantum analogue of
the Bohnenblust-Hille inequality

Back to the original talk

Learning to predict arbitrary quantum processes

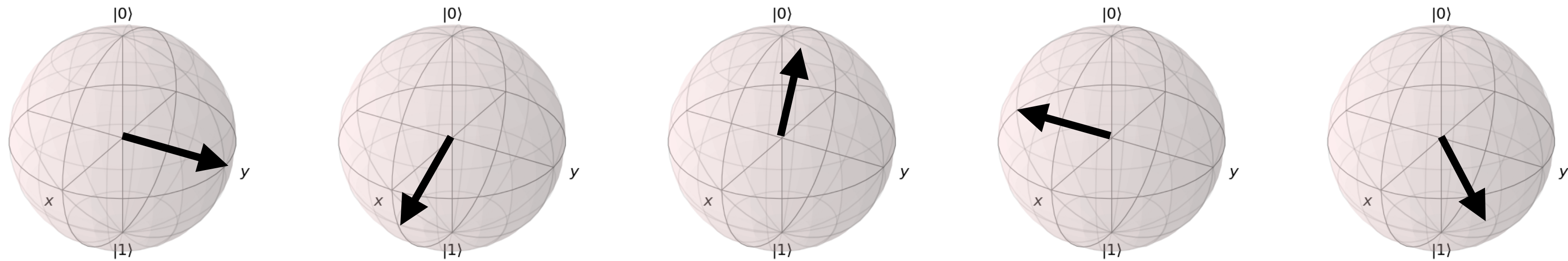
Presenter: Hsin-Yuan Huang (Robert)

Joint work with Sitan Chen and John Preskill



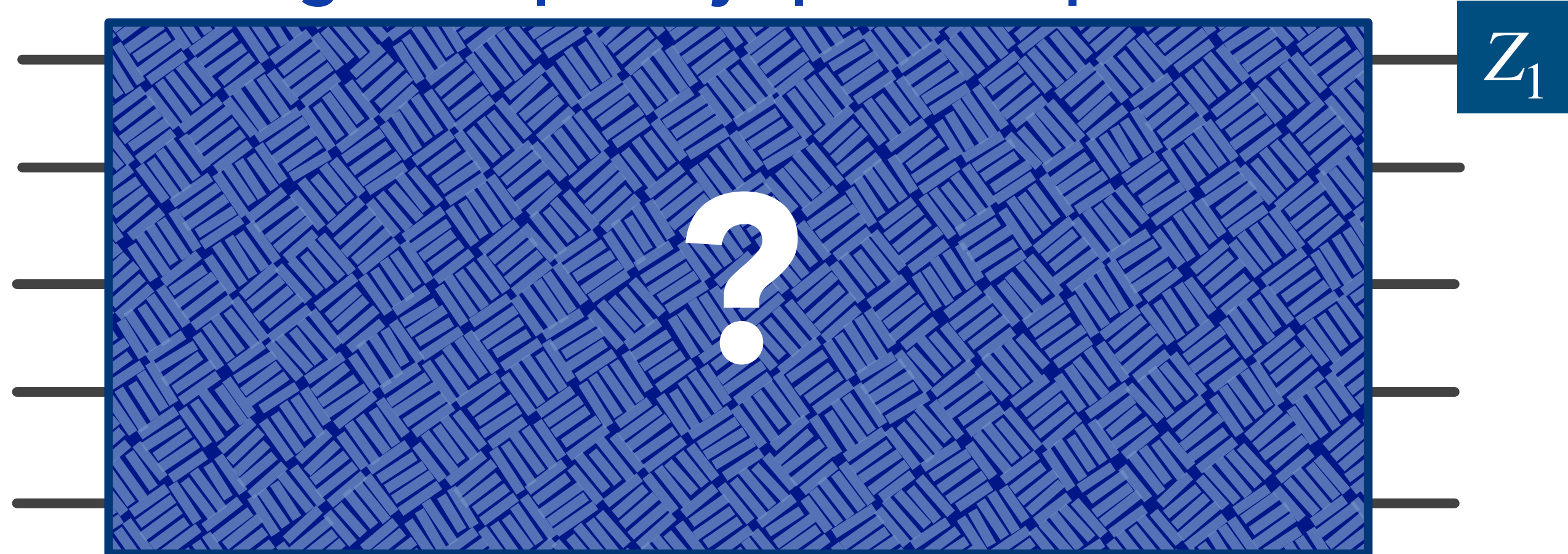
A Quantum Problem

Input:



A high-complexity quantum process

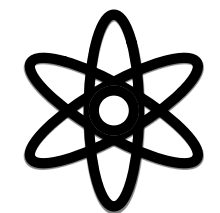
$$\bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$$



Basic Idea for the ML model

Basic idea: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Lemma (Fourier transform): $\alpha_P = \mathbb{E} \left[\frac{3^{|P|}}{N} \sum_{\ell=1}^N y_\ell \langle \psi_\ell | P | \psi_\ell \rangle \right], \forall P \in \{I, X, Y, Z\}^{\otimes n}$



Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

for $\ell = 1, \dots, N$.

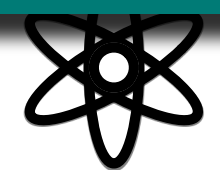
Basic Idea for the ML model

Basic idea: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Lemma

How large should the data size N be?

$\{X, Z\}^{\otimes n}$



Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

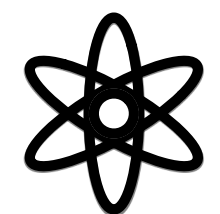
for $\ell = 1, \dots, N$.

Insight from Quantum BH inequality

Insight 1: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Insight 2: The Pauli coef. in $O^{(\text{low})}$ is approximately sparse as $\|\vec{\alpha}\|_{\frac{2k}{k+1}} \leq 2^{\mathcal{O}(k \log k)} \|O^{(\text{low})}\|_{\infty}$.

This idea is also used in classical learning theory [AI22]



Classical Dataset

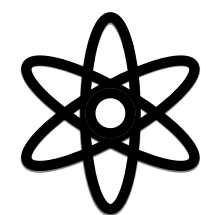
$$|\psi_{\ell}\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_{\ell}, \quad \mathbb{E}[y_{\ell}] = \langle \psi_{\ell} | O | \psi_{\ell} \rangle$$

for $\ell = 1, \dots, N$.

The ML algorithm

Insight 1: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Insight 2: The Pauli coef. in $O^{(\text{low})}$ is approximately sparse as $\|\vec{\alpha}\|_{\frac{2k}{k+1}} \leq 2^{\mathcal{O}(k \log k)} \|O^{(\text{low})}\|_{\infty}$.



Classical Dataset

$$|\psi_{\ell}\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_{\ell}, \quad \mathbb{E}[y_{\ell}] = \langle \psi_{\ell} | O | \psi_{\ell} \rangle$$

for $\ell = 1, \dots, N$.

For all $|P| \leq k$,

$$\text{set } \hat{\alpha}_P \leftarrow \frac{3^{|P|}}{N} \sum_{\ell=1}^N y_{\ell} \langle \psi_{\ell} | P | \psi_{\ell} \rangle.$$

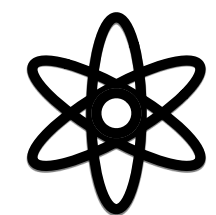
If $\hat{\alpha}_P$ is small, set $\hat{\alpha}_P \leftarrow 0$.

The learned observable is $\hat{O}^{(\text{low})} = \sum_{|P| \leq k} \hat{\alpha}_P P$.

Guarantee for learning $O^{(\text{low})}$

For any small constant ϵ , given a training set size $N = \mathcal{O}(\log n)$, the prediction error is

$$\mathbb{E}_{|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle} \left| \langle \psi | \hat{O}^{(\text{low})} | \psi \rangle - \langle \psi | O^{(\text{low})} | \psi \rangle \right|^2 < \epsilon \|O^{(\text{low})}\|_\infty^2.$$



Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

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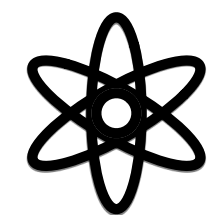
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Guarantee for learning O

For any small constant ϵ, ϵ' , given a training set size $N = \mathcal{O}(\log n)$, the prediction error is

$$\mathbb{E}_{|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle} \left| \langle \psi | \hat{O}^{(\text{low})} | \psi \rangle - \langle \psi | O | \psi \rangle \right|^2 < \epsilon + \epsilon' \|O^{(\text{low})}\|_{\infty}^2.$$



Classical Dataset

$$|\psi_{\ell}\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_{\ell}, \quad \mathbb{E}[y_{\ell}] = \langle \psi_{\ell} | O | \psi_{\ell} \rangle$$

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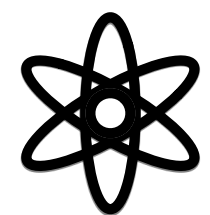
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Guarantee for learning O

For any ϵ, ϵ' , given a training set size $N = \log(n) 2^{\tilde{O}(\log(1/\epsilon)\log(1/\epsilon'))}$, the prediction error is

$$\mathbb{E}_{|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle} \left| \langle \psi | \hat{O}^{(\text{low})} | \psi \rangle - \langle \psi | O | \psi \rangle \right|^2 < \epsilon + \epsilon' \|O^{(\text{low})}\|_{\infty}^2.$$



Classical Dataset

$$|\psi_{\ell}\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_{\ell}, \quad \mathbb{E}[y_{\ell}] = \langle \psi_{\ell} | O | \psi_{\ell} \rangle$$

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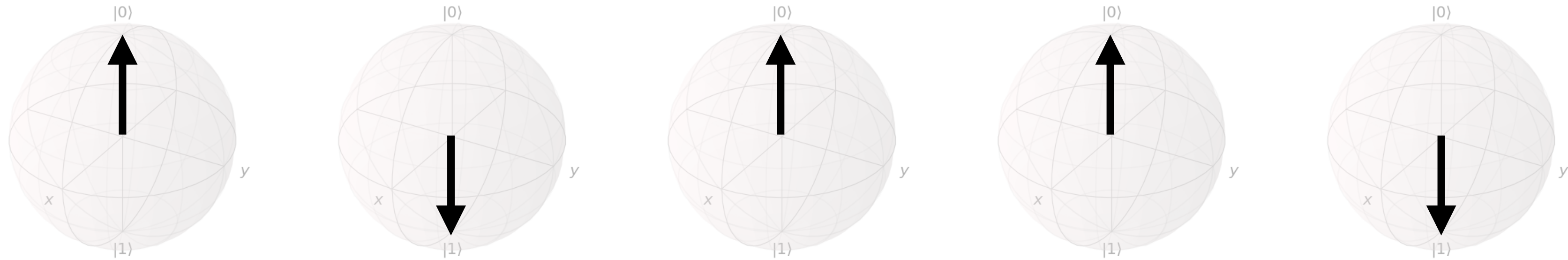
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A Classical Problem

Input:



A high-complexity classical circuit

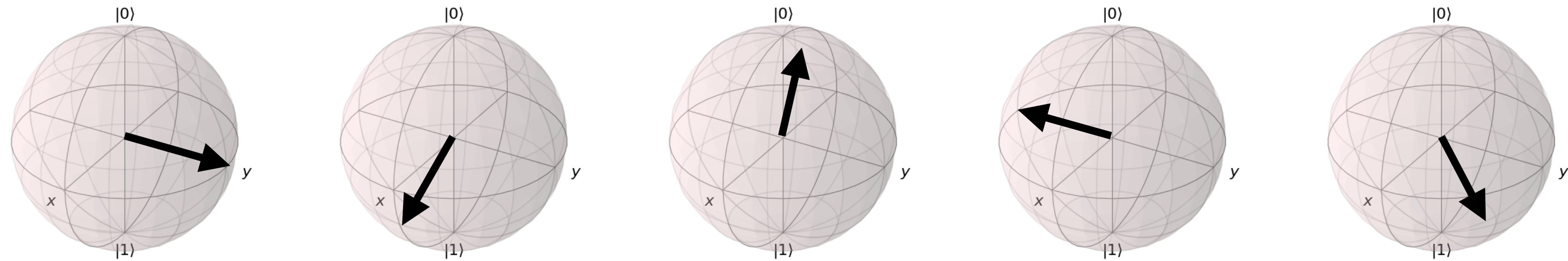
$$x \in \{-1, 1\}^n$$



**Exponentially
hard!**

A Quantum Problem

Input:



A high-complexity quantum process

$$\bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$$



Quasi-polynomially
easy!

Overview

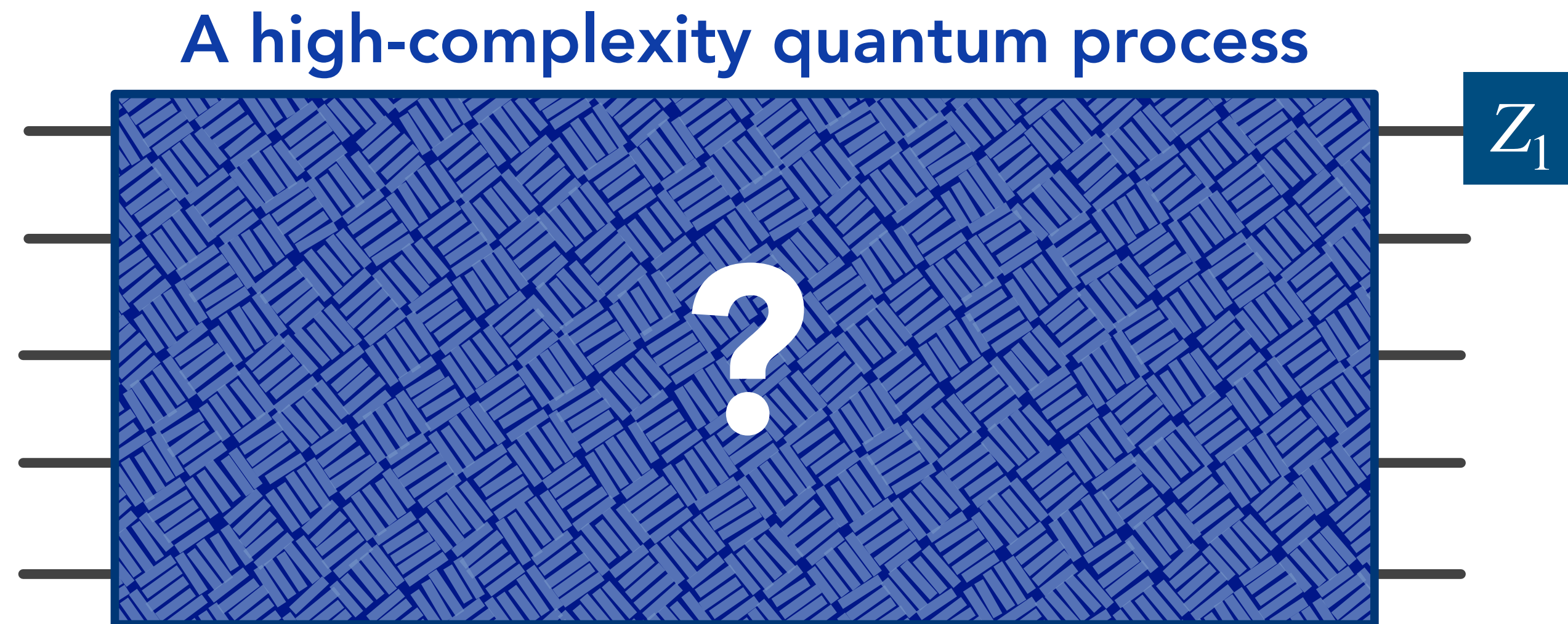
- A classical version of the quantum problem
- A restricted version of the quantum problem
- Generalization to the original quantum problem

Overview

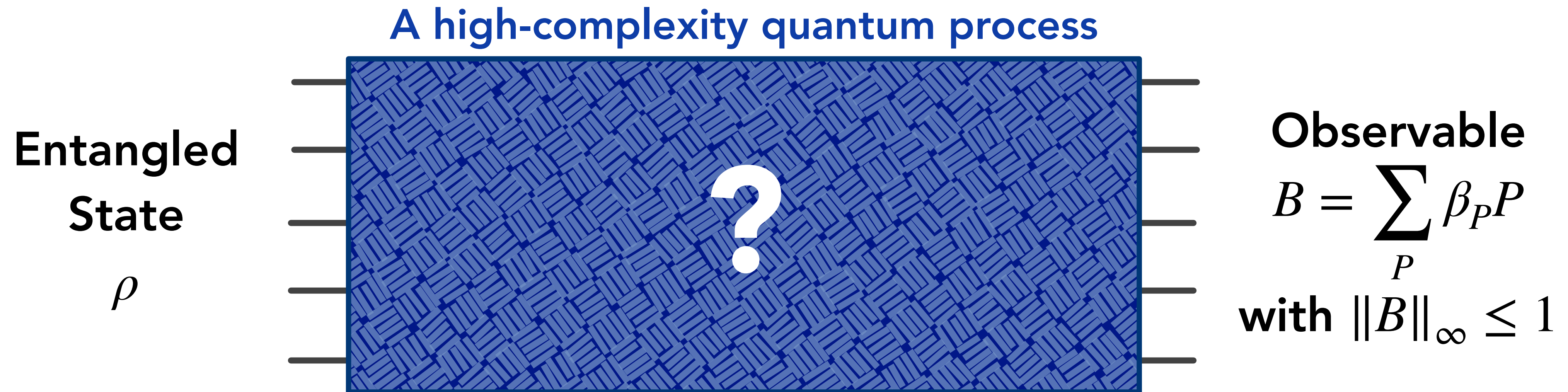
- A classical version of the quantum problem
- A restricted version of the quantum problem
- Generalization to the original quantum problem

The Restricted Problem

$$\bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$$

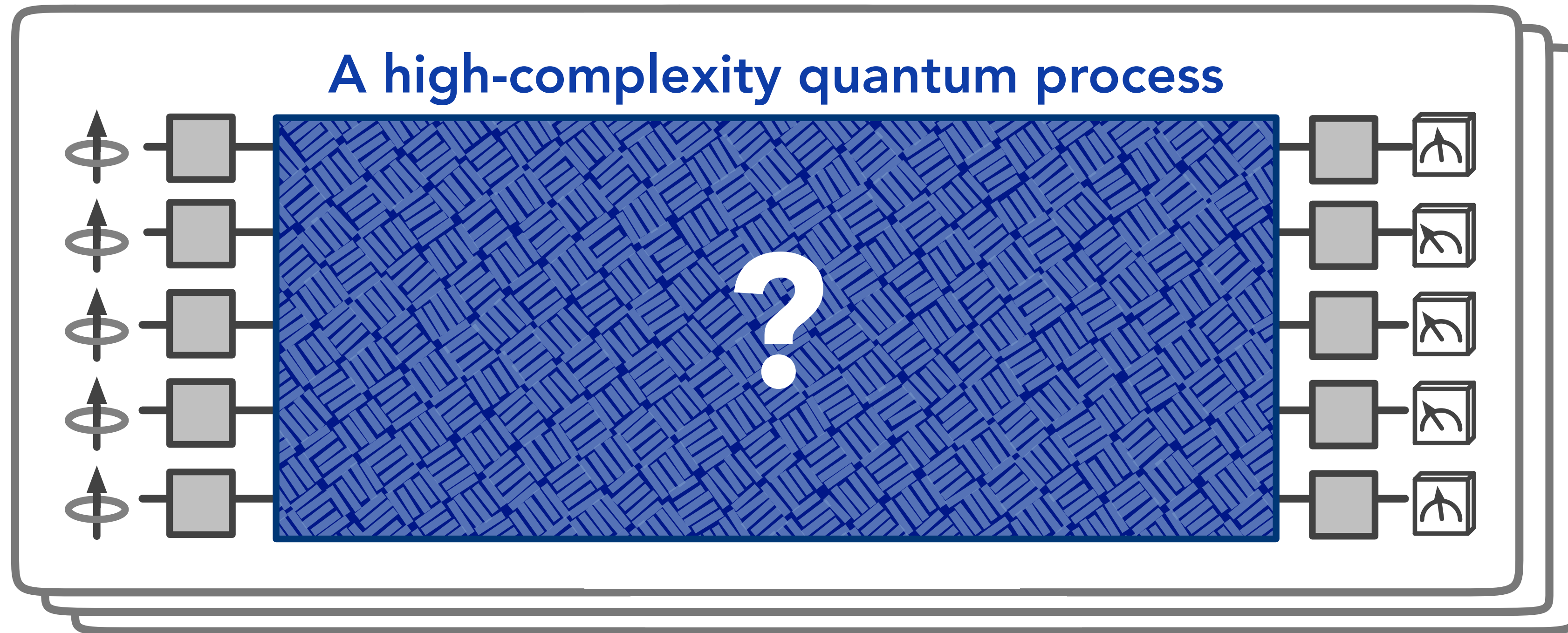


The Original Problem



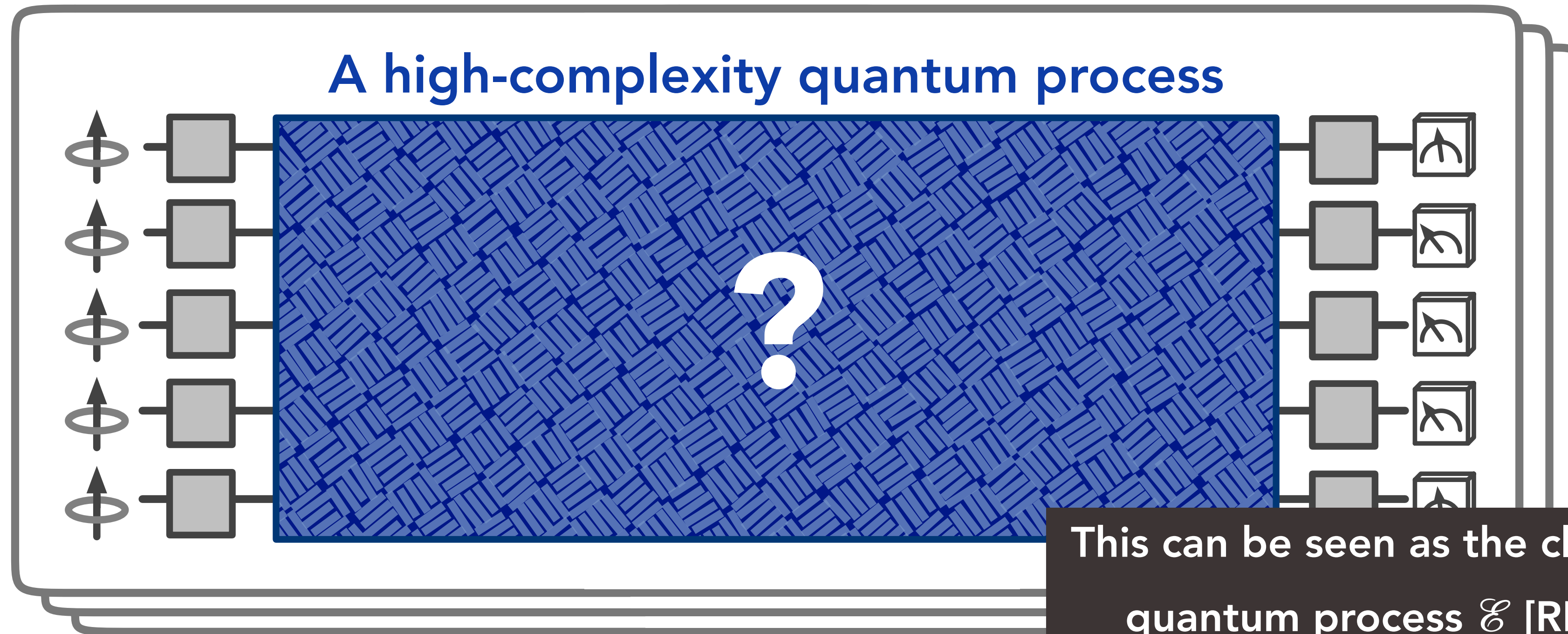
A Classical Dataset for Learning \mathcal{E}

Some Repetitions

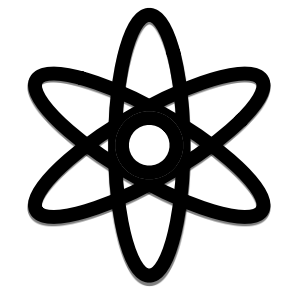


A Classical Dataset for Learning \mathcal{E}

Some Repetitions



A Classical Dataset for Learning \mathcal{E}



Classical Dataset

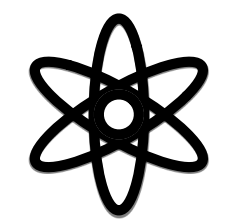
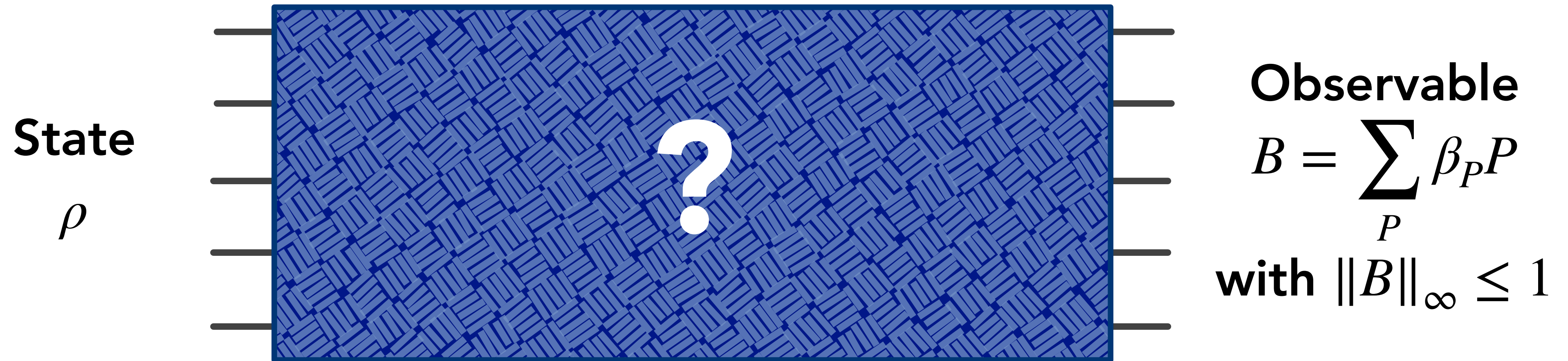
$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto |\phi_\ell\rangle = \bigotimes_{i=1}^n |\phi_{\ell,i}\rangle$$

for $\ell = 1, \dots, N$.

This can be seen as the classical shadow of quantum process \mathcal{E} [RLC21, KTC+21]

How to make prediction?

A high-complexity quantum process

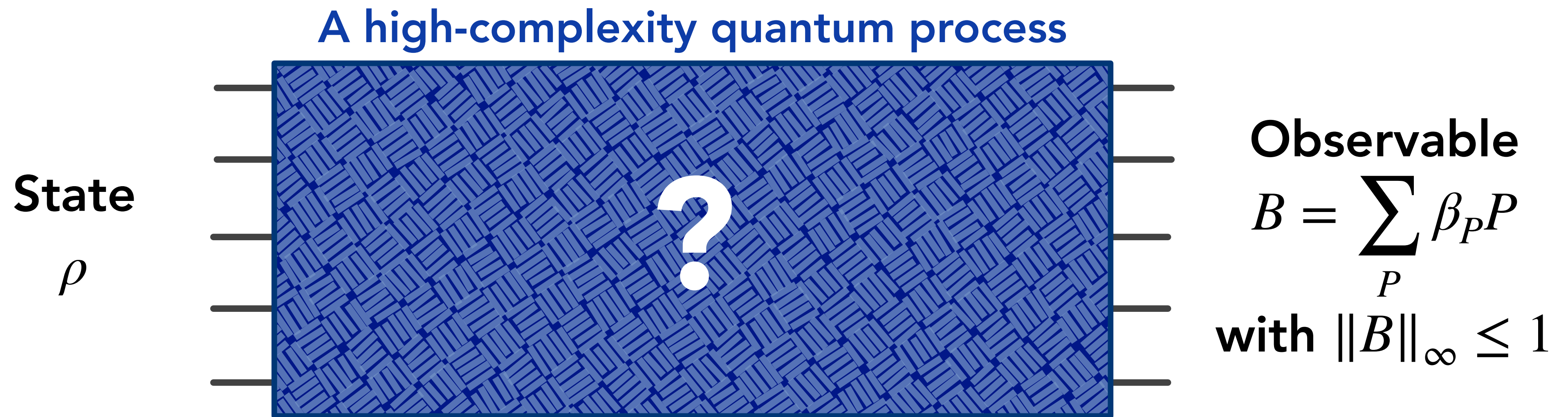


Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto |\phi_\ell\rangle = \bigotimes_{i=1}^n |\phi_{\ell,i}\rangle$$

for $\ell = 1, \dots, N$.

Construct a dataset with classical shadow



A New Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell = \text{Tr} \left(B \bigotimes_{i=1}^n (3|\phi_{\ell,i}\rangle\langle\phi_{\ell,i}| - I) \right)$$

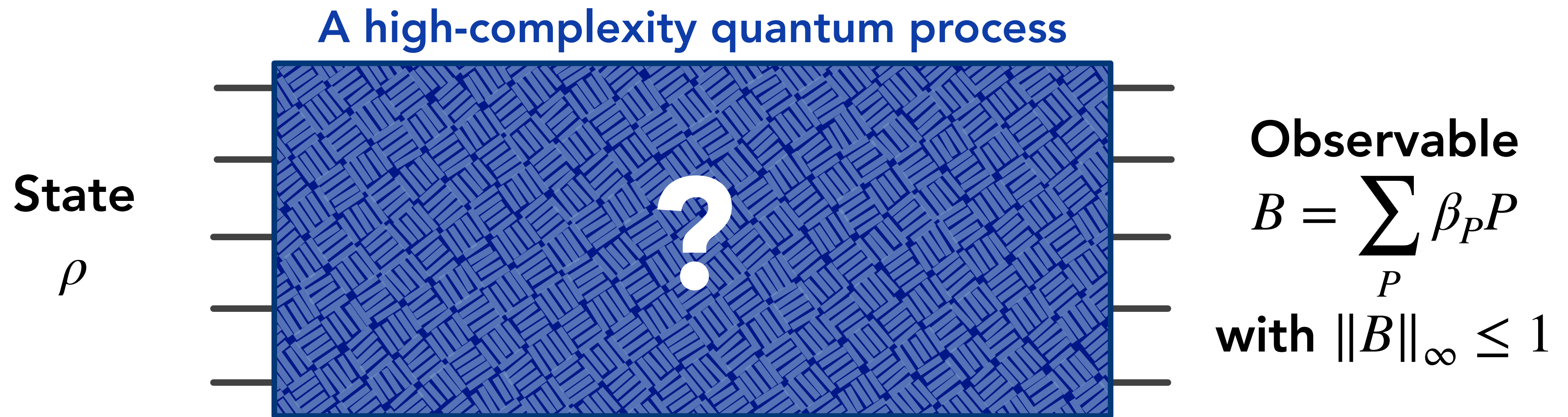
for $\ell = 1, \dots, N$.

Properties [HKP20]:

$$\mathbb{E}[y_\ell] = \text{Tr}(B \mathcal{E}(|\psi_\ell\rangle\langle\psi_\ell|))$$

$$\text{Var}[y_\ell] \leq \|B\|_{\text{shadow}}^2$$

Construct a dataset with classical shadow



A New Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell = \text{Tr} \left(B \bigotimes_{i=1}^n (3|\phi_{\ell,i}\rangle\langle\phi_{\ell,i}| - I) \right)$$

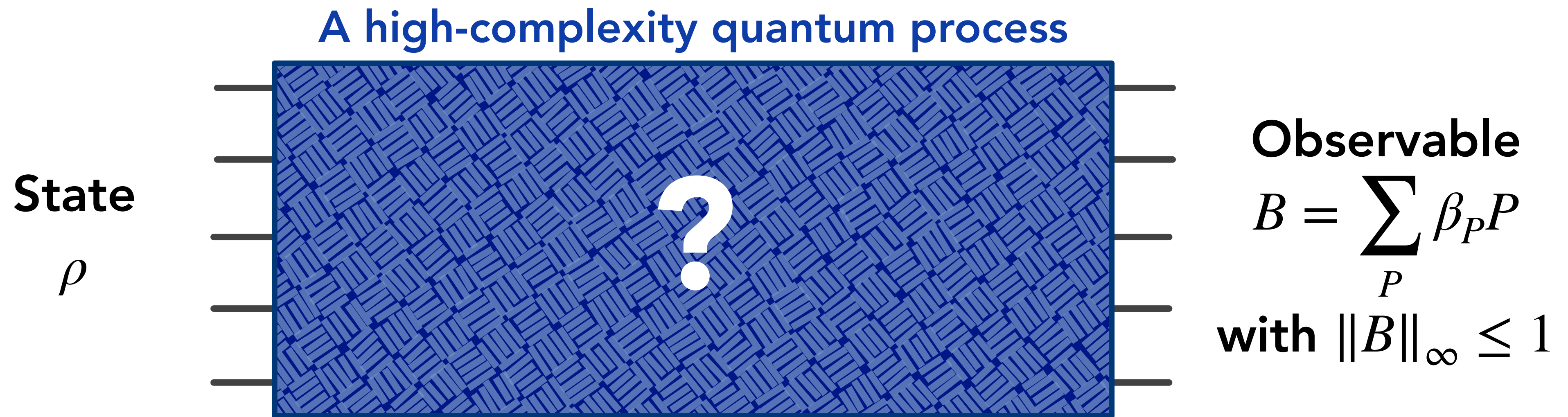
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Construct a dataset with classical shadow



For any sum of local observables B , $\|B\|_{\text{shadow}} \leq \mathcal{O}(\|\vec{\beta}\|_1) \leq \mathcal{O}(\|B\|_\infty)$
using the generalized quantum BH inequality.

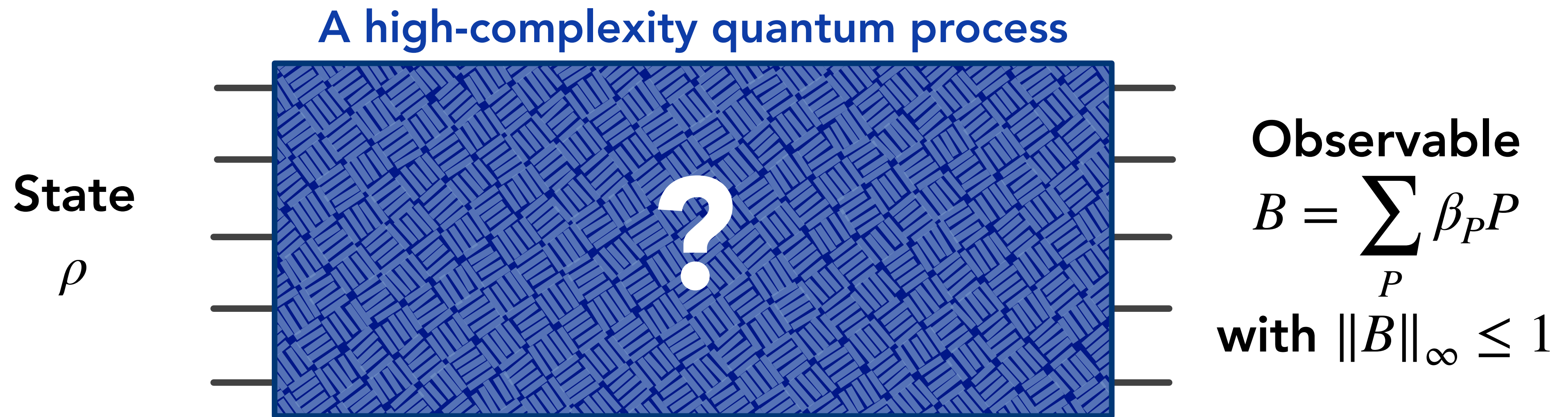
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for $\ell = 1, \dots, N$.

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Construct a dataset with classical shadow



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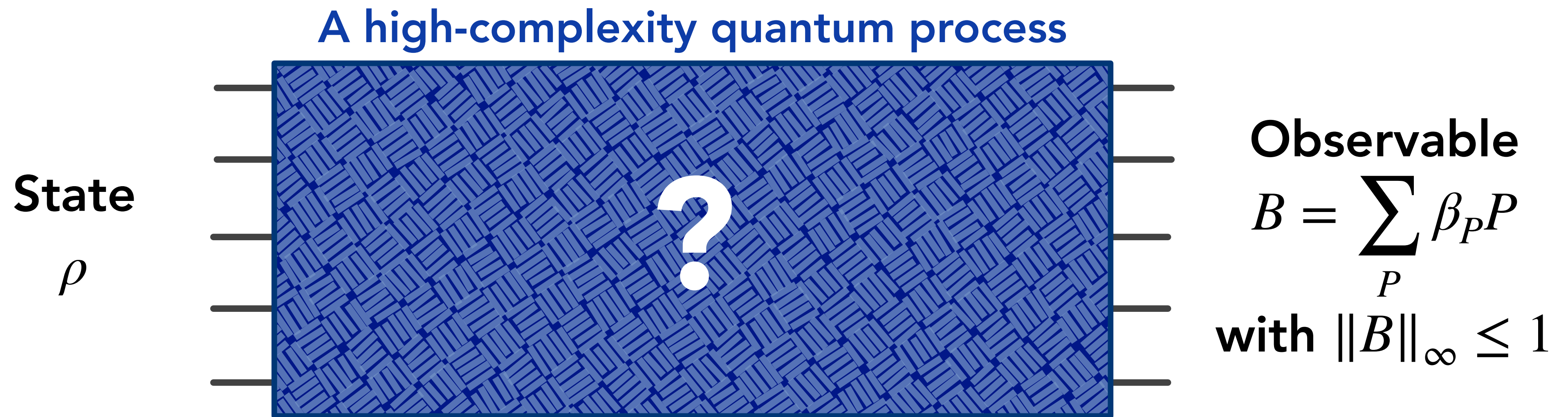
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for $\ell = 1, \dots, N$.

$$\mathbb{E}[y_\ell] = \text{Tr}(B \mathcal{E}(|\psi_\ell\rangle\langle\psi_\ell|))$$

$$\text{Var}[y_\ell] = \mathcal{O}(1)$$

Construct a dataset with classical shadow



A New Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell = \text{Tr} \left(B \bigotimes_{i=1}^n (3|\phi_{\ell,i}\rangle\langle\phi_{\ell,i}| - I) \right)$$

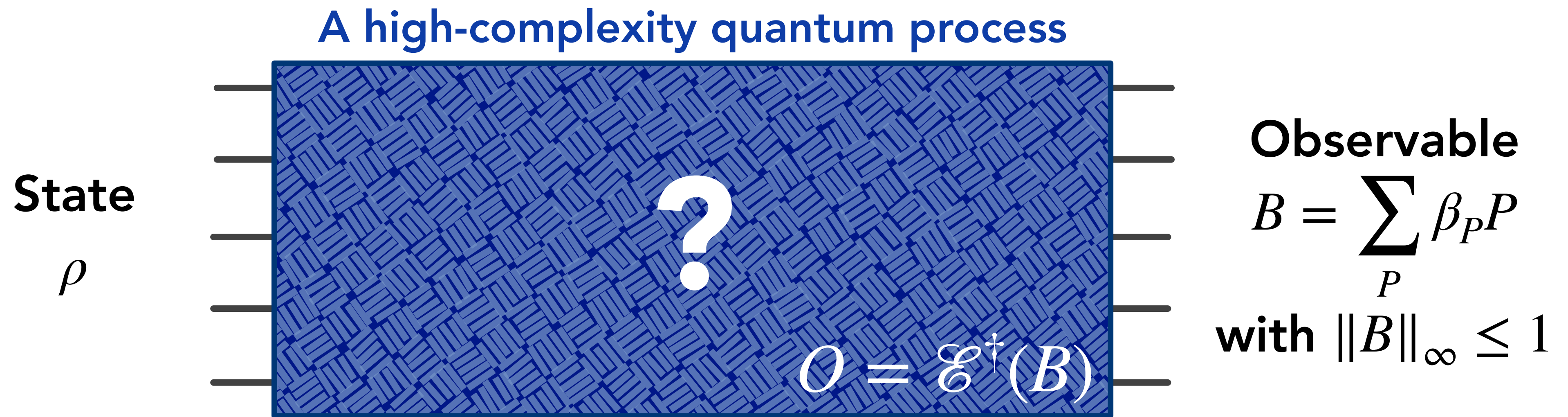
for $\ell = 1, \dots, N$.

Properties [HKP20]:

$$\mathbb{E}[y_\ell] = \text{Tr}(B \mathcal{E}(|\psi_\ell\rangle\langle\psi_\ell|))$$

$$\text{Var}[y_\ell] = \mathcal{O}(1)$$

Almost back to the previous problem



✱ Classical Dataset for O

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

for $\ell = 1, \dots, N$.

Low-weight approximation

$$O = \sum_{P \in \{I, X, Y, Z\}^{\otimes n}} \alpha_P P$$

$$O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$$

Lemma (Low-weight approximation): $\mathbb{E}_{\rho \sim \mathcal{D}} \left| \text{Tr}(O\rho) - \text{Tr}(O^{(\text{low})}\rho) \right|^2 < \frac{1}{1.5^k}$.

The lemma holds for any distribution \mathcal{D} over any quantum state ρ as long as \mathcal{D} is flat under single-qubit rotations.

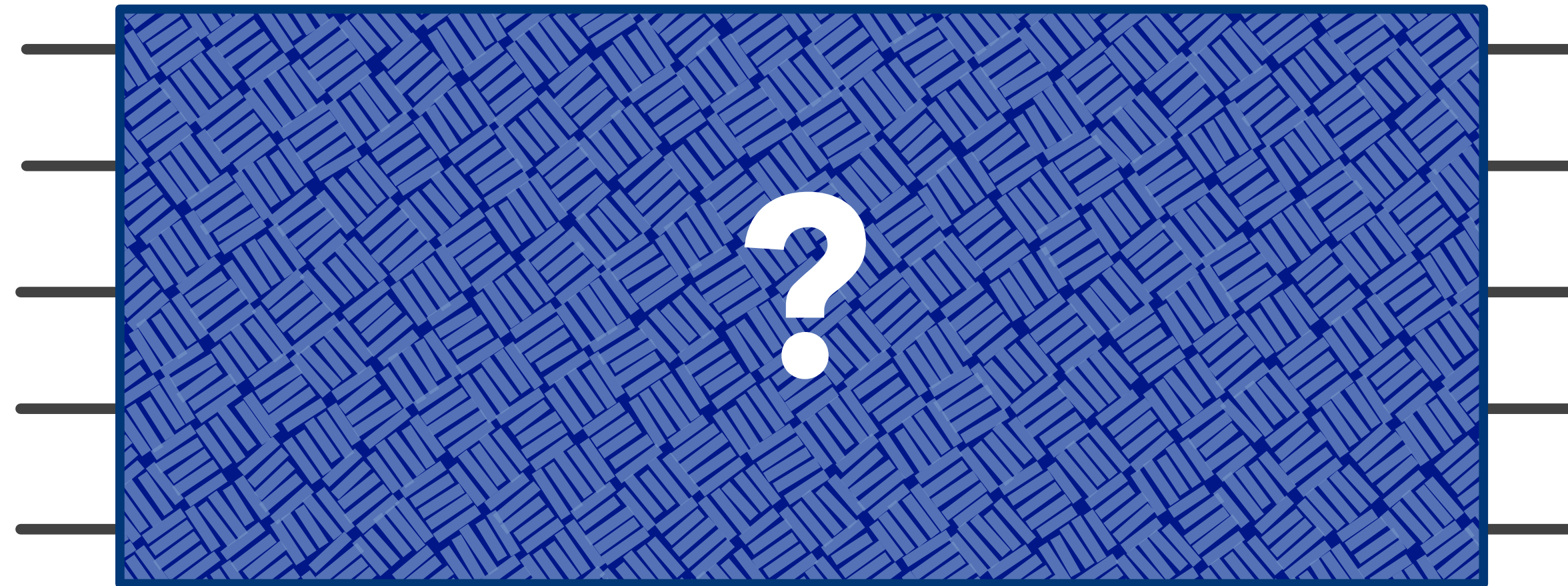
Example: ρ is the ground/thermal state of a generic geometrically-local Hamiltonian.

The ML algorithm

A high-complexity quantum process

State

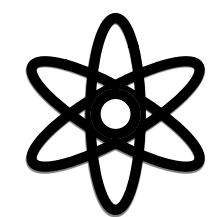
ρ



Observable

$$B = \sum_P \beta_P P$$

with $\|B\|_\infty \leq 1$

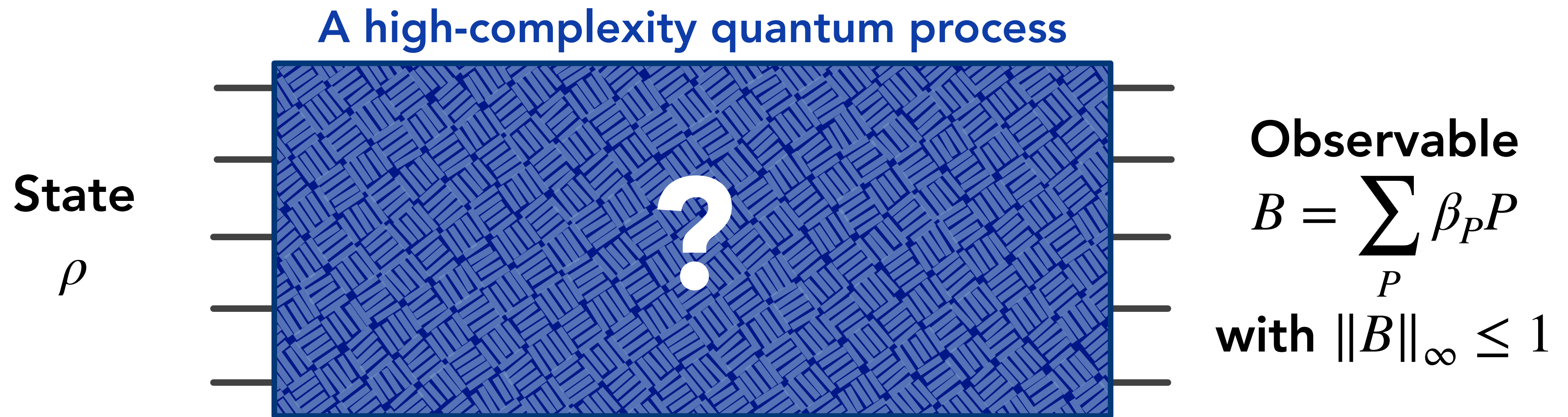


Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto |\phi_\ell\rangle = \bigotimes_{i=1}^n |\phi_{\ell,i}\rangle$$

for $\ell = 1, \dots, N$.

The ML algorithm



✱ Classical Dataset for $O = \mathcal{E}^\dagger(B)$

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

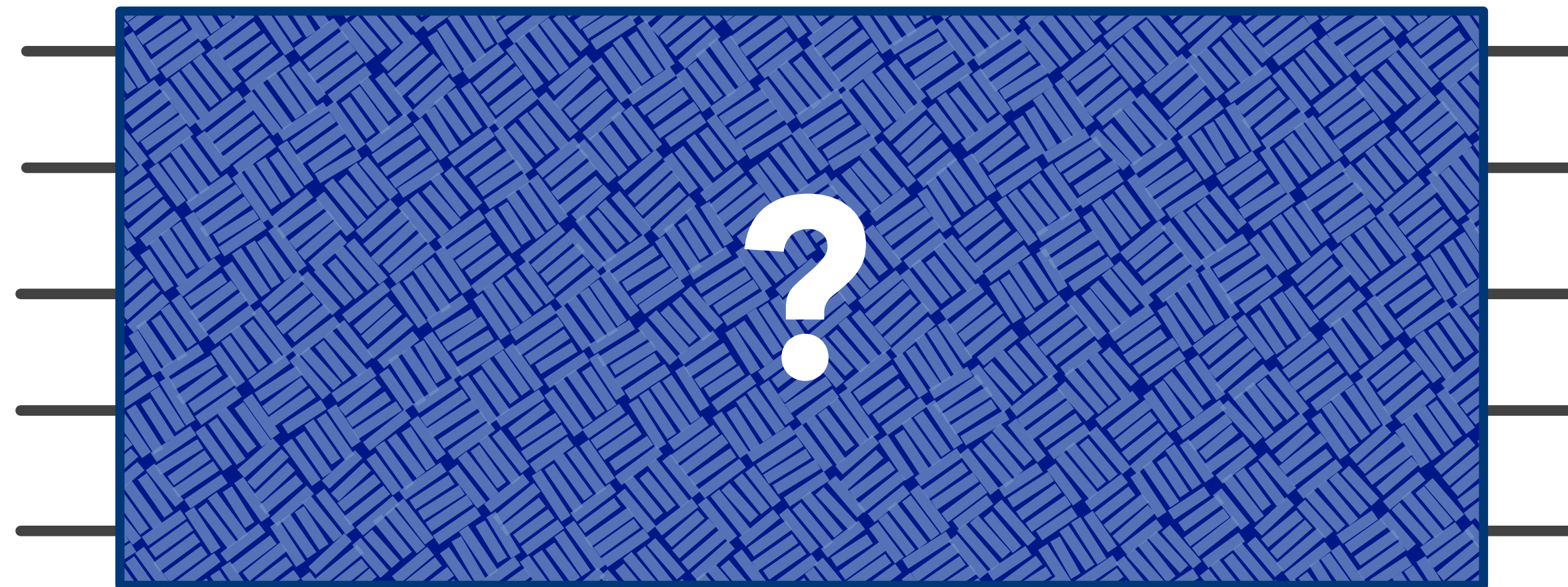
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The ML algorithm

A high-complexity quantum process

State

ρ



Observable

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For all $|P| \leq k$,

$$\text{set } \hat{\alpha}_P \leftarrow \frac{3^{|P|}}{N} \sum_{\ell=1}^N y_\ell \langle \psi_\ell | P | \psi_\ell \rangle.$$

If $\hat{\alpha}_P$ is small, set $\hat{\alpha}_P \leftarrow 0$.

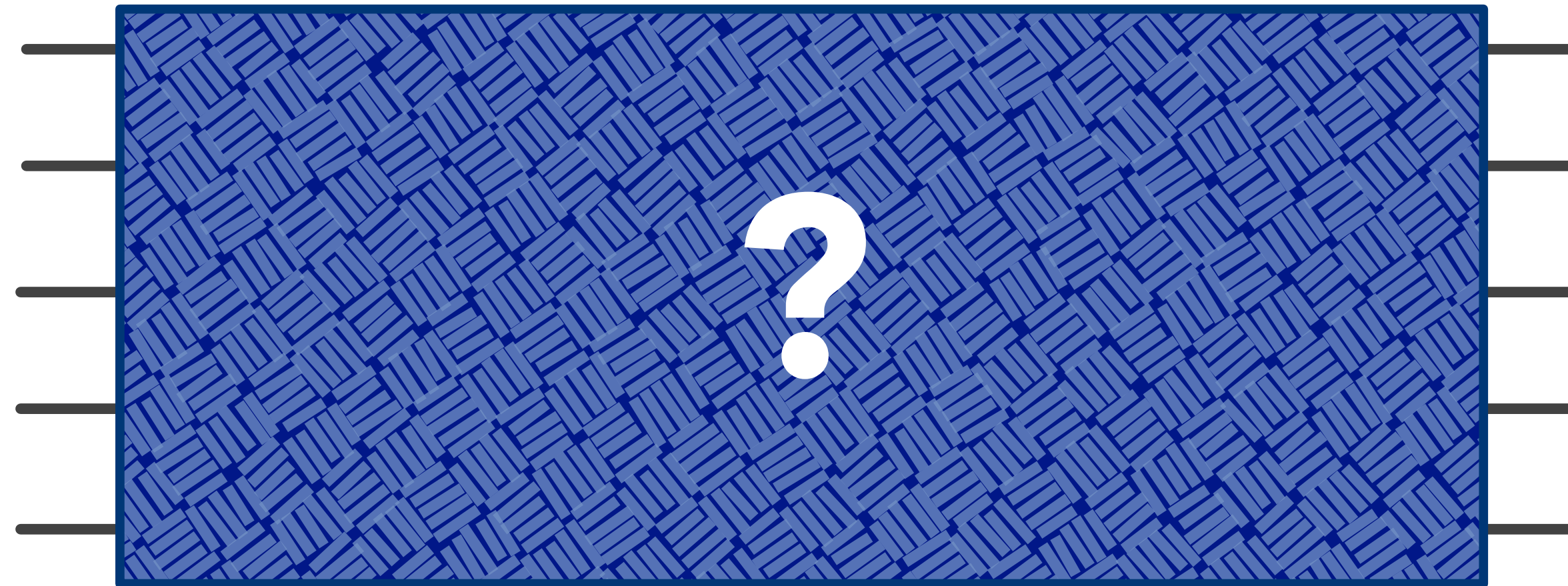
The learned observable is $\hat{O}^{(\text{low})} = \sum_{|P| \leq k} \hat{\alpha}_P P$.

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$$\text{Predict } \text{Tr} \left(\hat{O}^{(\text{low})} \rho \right) \approx \text{Tr} \left(B \mathcal{E}(\rho) \right)$$

Surprising aspects of the ML algorithm

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- After learning from product state inputs, the algorithm can predict entangled states.
- The entire algorithm can be run on a classical computer.

Conclusion

- We give a computationally-efficient ML algorithm that can learn to predict the output of a quantum process with arbitrary complexity.
- Our results highlight the potential that ML models can predict outcomes of a complex quantum dynamics much faster than the process itself.

