Neural quantum state tomography

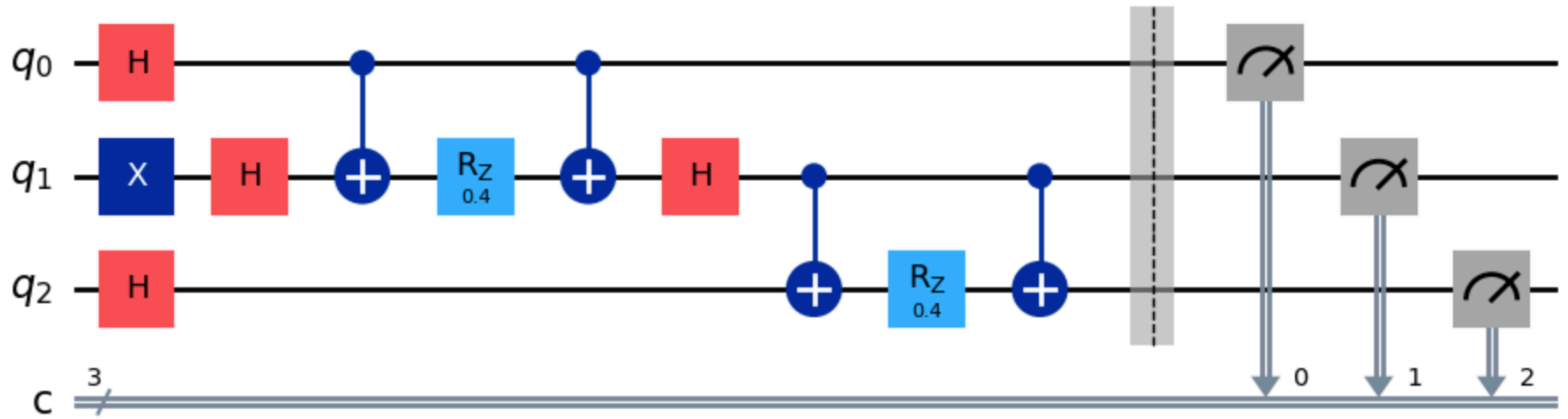
Shunji Matsuura

with/ Wirawat Kokaew, Bohdan Kulchytskyy, Pooya Ronagh

arXiv:2405.06864

Quantum states in quantum computing

Typical quantum circuit



Quantum computing is powerful
because it does massive parallel computing

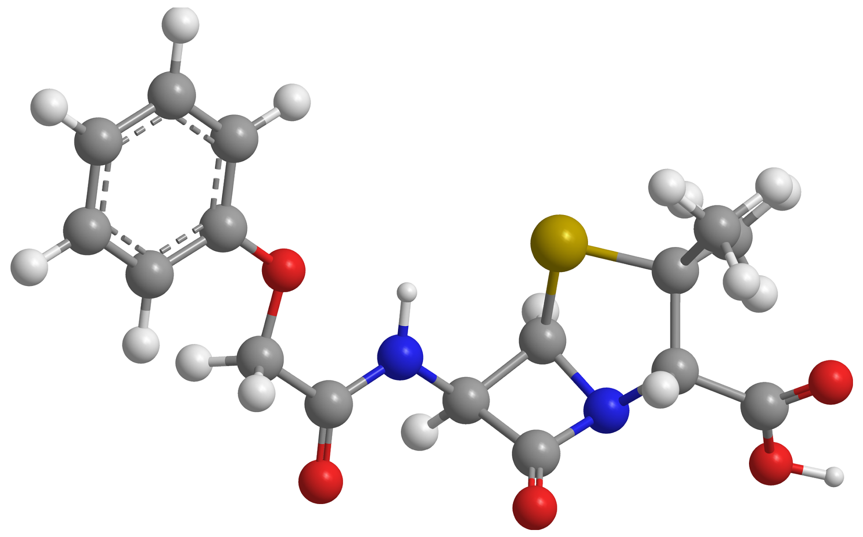
$$|\psi\rangle = \sum_{k=1}^{2^n} a_k |k\rangle$$

Measurement:
Exponential information loss!

$$|k\rangle$$

Challenge of quantum measurements

Chemistry



$$H = \sum f_{ij} a_i^\dagger a_j + \sum f_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

$$\rightarrow \sum_k \tilde{f}_k P_k \quad (P_k : \text{Pauli operators})$$

Energy $\quad E = \langle H \rangle = \sum_k \tilde{f}_k \langle P_k \rangle$

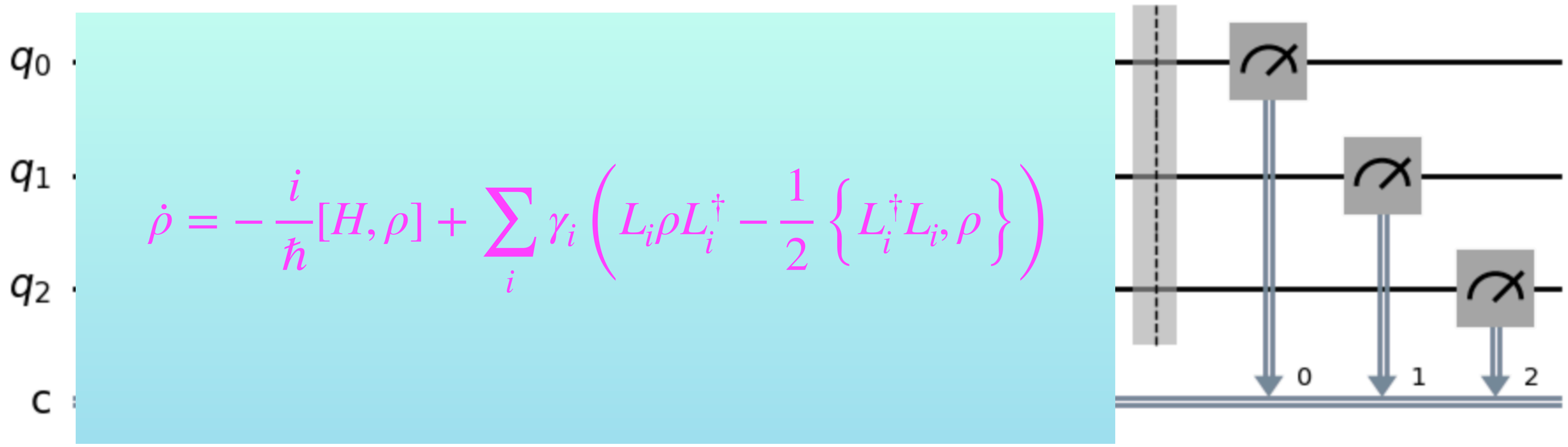
Hydrogen atom

$P_k =$ ['IIII', 'IIIZ', 'IIZI', 'IIZZ', 'IZII', 'IZIZ', 'ZIII', 'ZIIZ', 'IZZI', 'ZIZI', 'ZZII', 'YYYY', 'XXYY', 'YYXX', 'XXXX',]

n-qubit: $|P| \sim \mathcal{O}(n^4)$,

# of measurements$=N$: Sampling error $\sim 1/\sqrt{N}$

Unknown quantum evolution



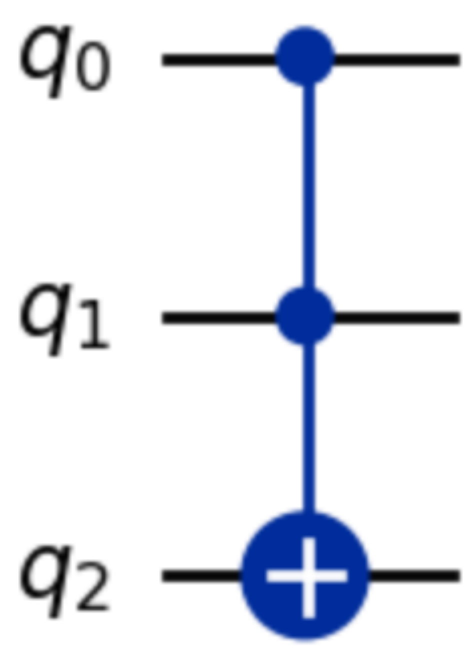
Is the final state entangled or separable?

$$\text{For a Hermitian operator } A \begin{cases} \text{Entangled state } \rightarrow \mathrm{Tr}(A\rho) < 0 \\ \mathrm{Tr}(A\rho) \geq 0 \rightarrow \text{Separable state} \end{cases}$$

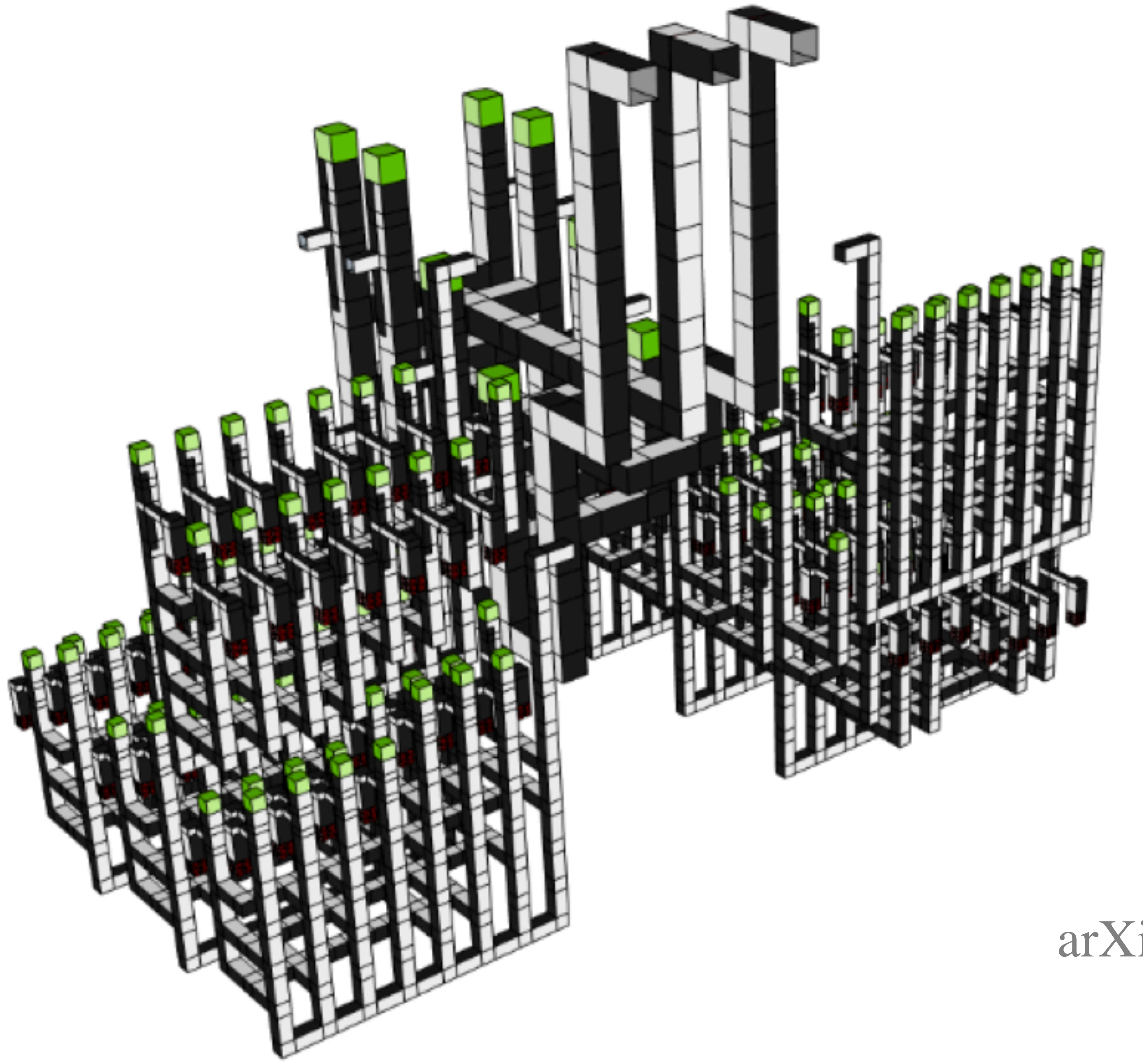
However $|\mathrm{Tr}\,(A\rho)|$ can be very small: Sensitive to sampling error

Fault tolerant quantum computing

Significant overhead



NISQ

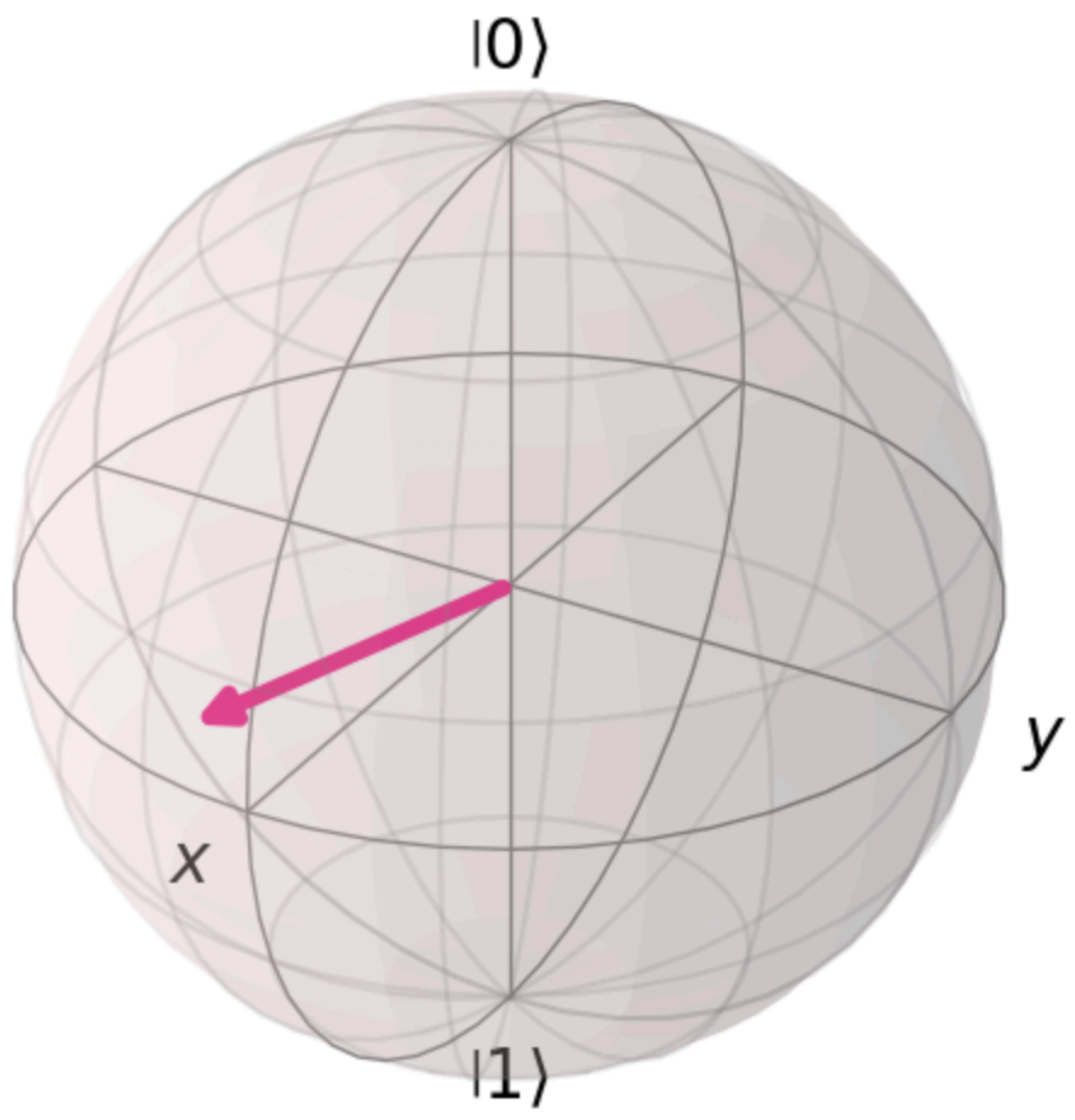


arXiv:2011.04149

FTQC

Reducing measurement complexity is useful in FTQC too!

State Tomography



$$\rho = \frac{1}{2}\left(I + a_x X + a_y Y + a_z Z\right)$$

$$a_x = \mathrm{tr}\left(\rho X\right) = \langle X \rangle$$

$$a_y = \mathrm{tr}\left(\rho Y\right) = \langle Y \rangle$$

$$a_z = \mathrm{tr}\left(\rho Z\right) = \langle Z \rangle$$

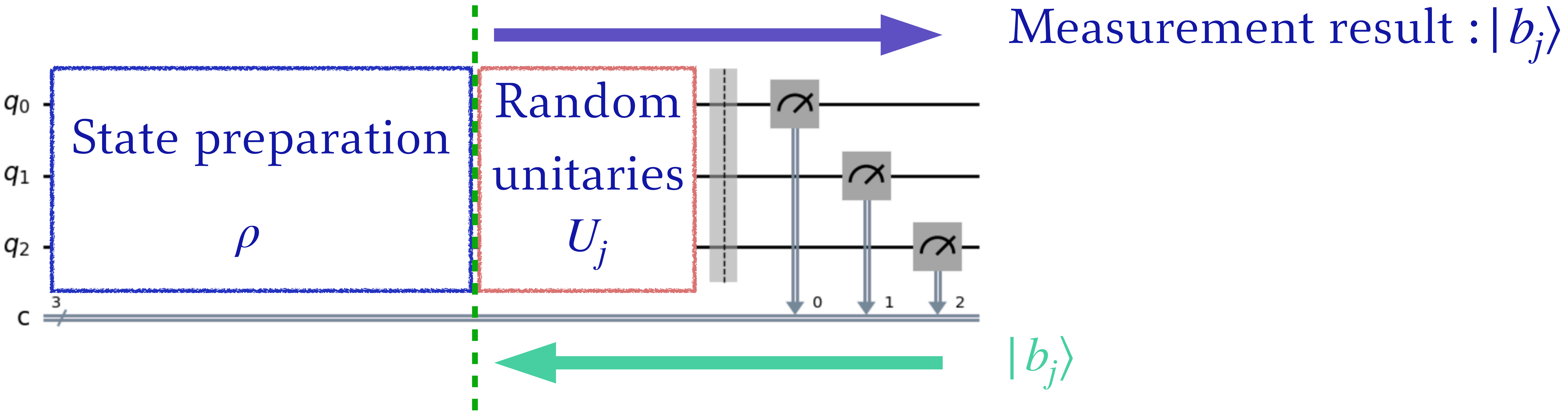
Multi-qubit case

Measure all possible Paulis (4^n)

$$\langle IXIZ \rangle, \langle YYZX \rangle, \ldots$$

Classical Shadow Tomography

[Huang-Kueng-Preskill '20]



$$\rho \neq U_j^\dagger |b_j\rangle\langle b_j| U_j$$

$$\mathcal{M}(\rho) = \mathbb{E}\left[U_j^\dagger |b_j\rangle\langle b_j| U_j\right]$$

$$\rho = \mathbb{E}\left[\mathcal{M}^{-1}\left(U_j^\dagger |b_j\rangle\langle b_j| U_j\right)\right]$$

Classical Shadow Tomography

$$\hat{\rho}_i = \mathscr{M}^{-1}\left[U_i^\dagger |b_i\rangle\langle b_i| U_i\right]$$

$$\mathbb{E}(\hat{\rho}) = \rho$$

$$\langle O_a \rangle = \frac{1}{K}\sum_{i=1}^{K} \mathrm{tr}\left(\hat{\rho}_i O_a\right)$$

If we want to estimate M observables with accuracy ϵ,

Sampling complexity : $K = \mathcal{O}(\boxed{\log(M)} \max_i \|O_i\|^2_{\mathrm{shadow}}/\epsilon^2)$

Exponentially efficient

Classical Shadow Tomography

However, each $\hat{\rho}$ is not necessarily physical

For instance, if we measure $|0\rangle \Rightarrow \hat{\rho} = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}$

Suppose we want to compute the entanglement entropy

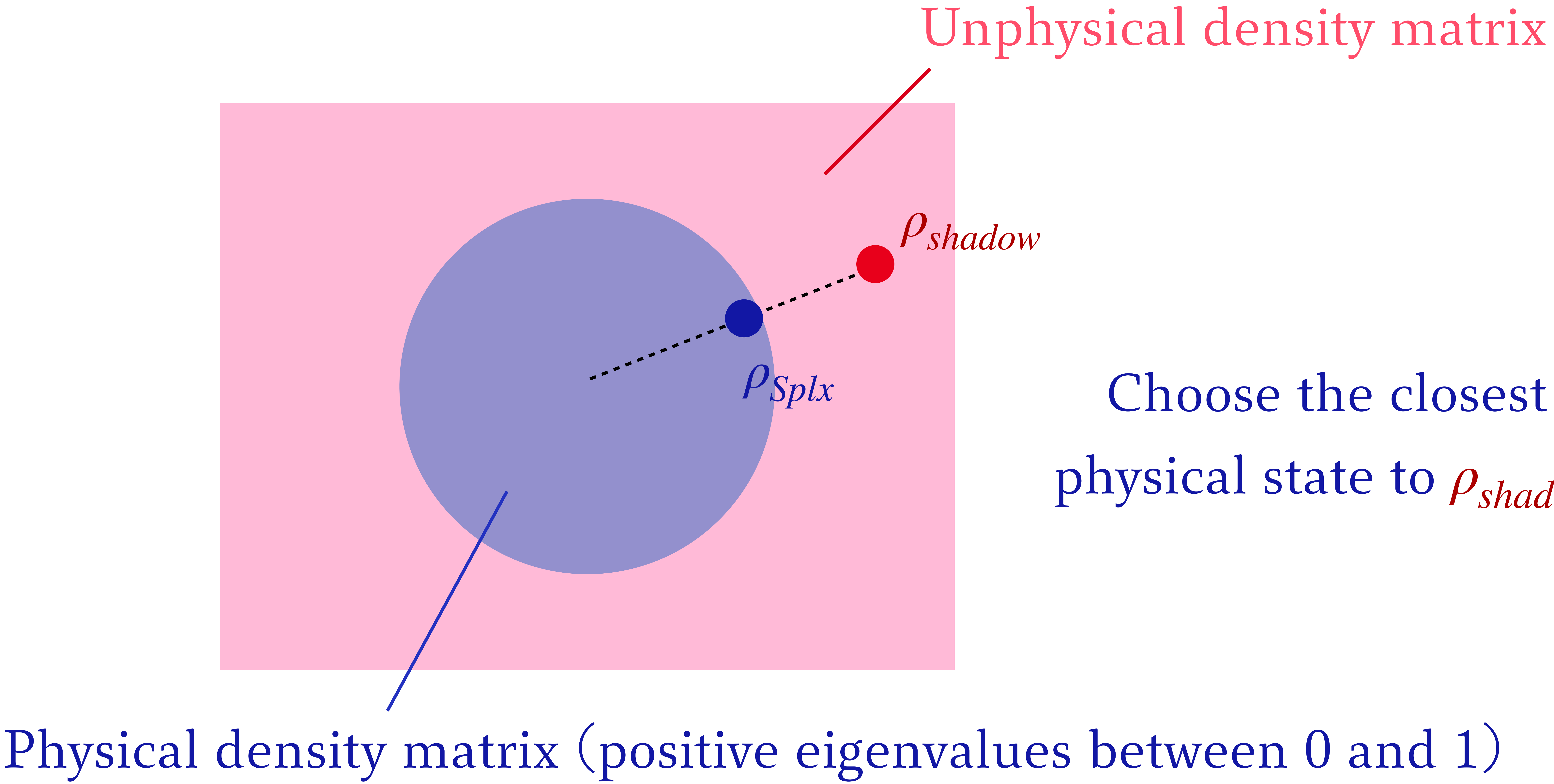
(🛑 This is just for intuition, sampling number = 1)

“ $S = -\operatorname{tr}\left(\rho \log \rho\right)$ ”

$= -(2\log 2 + (-1)\log(-1))$

Ill-defined

Solution 1 : Simplex projection



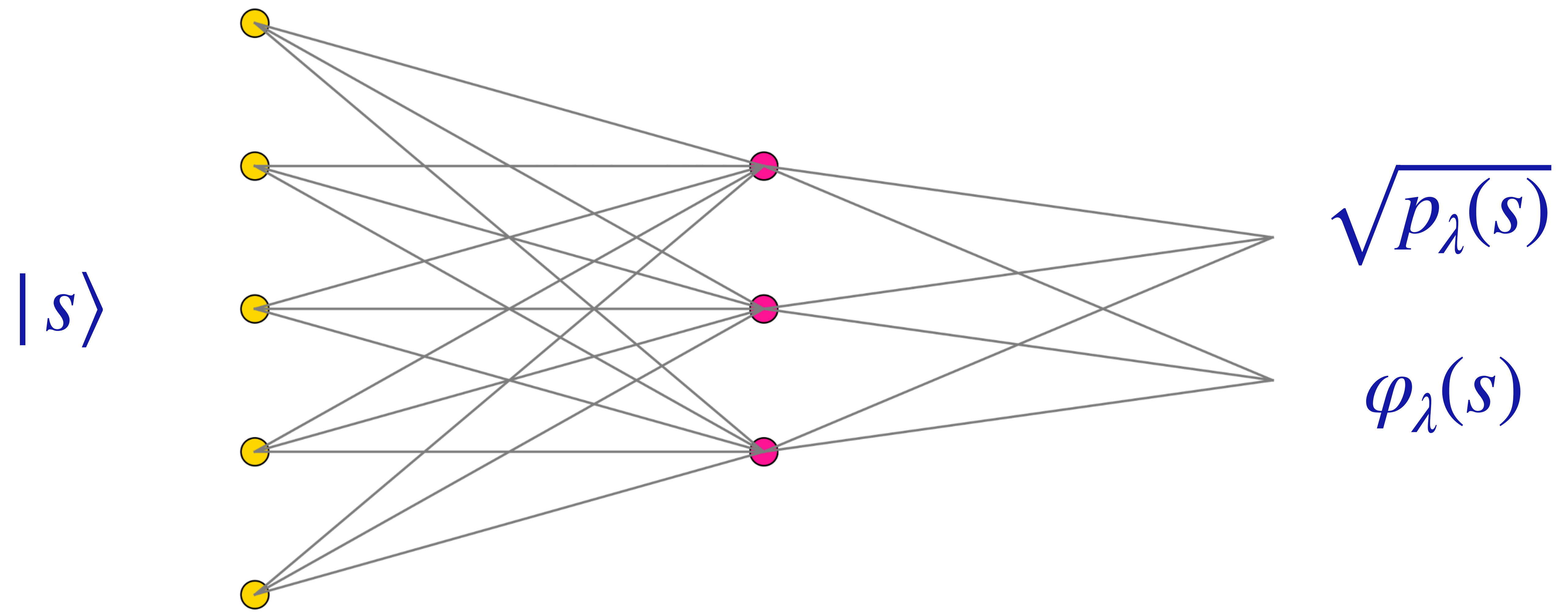
Choose the closest physical state to ρ_{shadow}

Solution 2 : Neural network quantum state

[Torlai-Mazzola-Carrasquilla-Troyer-Melko-Carleo '18, Carrasquilla-Torlai-Melko-Aolita '19]

$$|\psi\rangle = \sum_s \sqrt{p_\lambda(s)} e^{i\varphi_\lambda(s)} |s\rangle$$

Computational basis

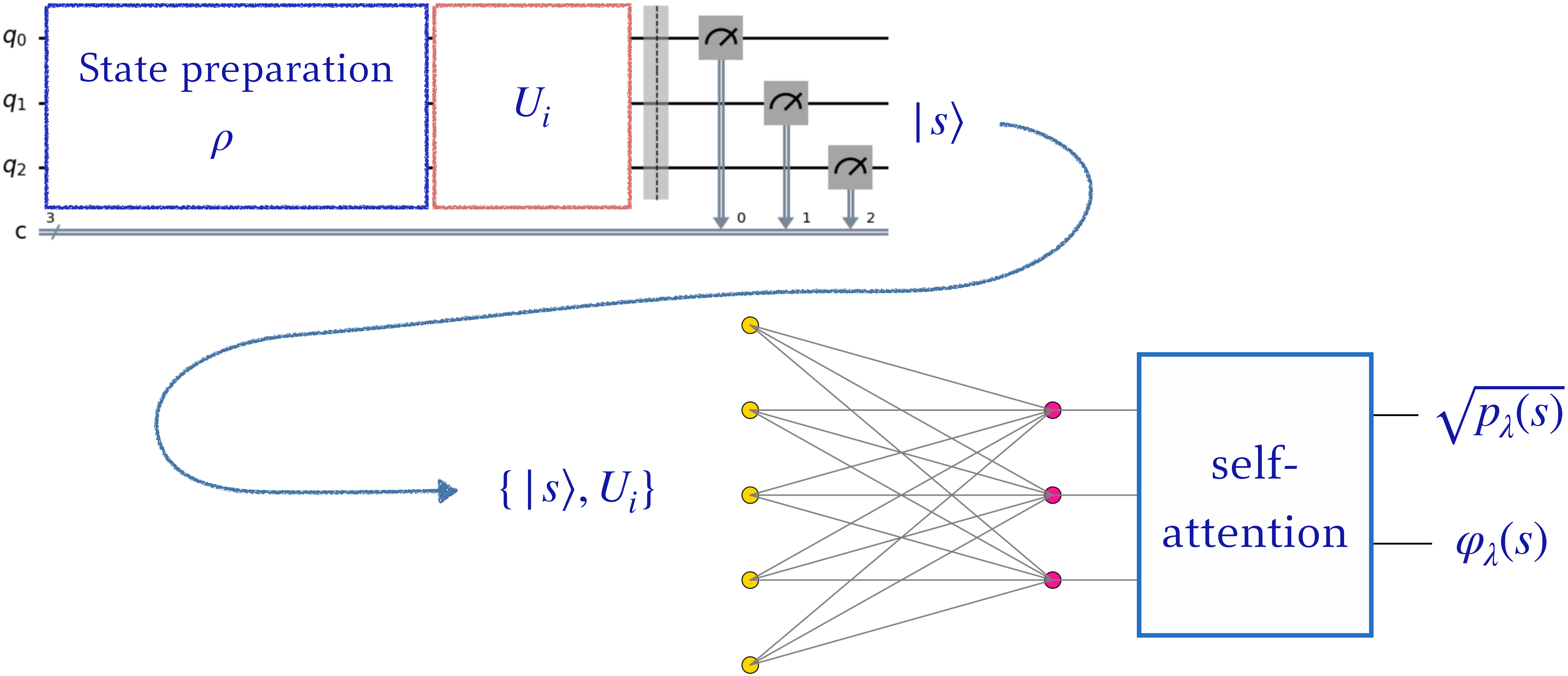


Neural network

parametrized by λ

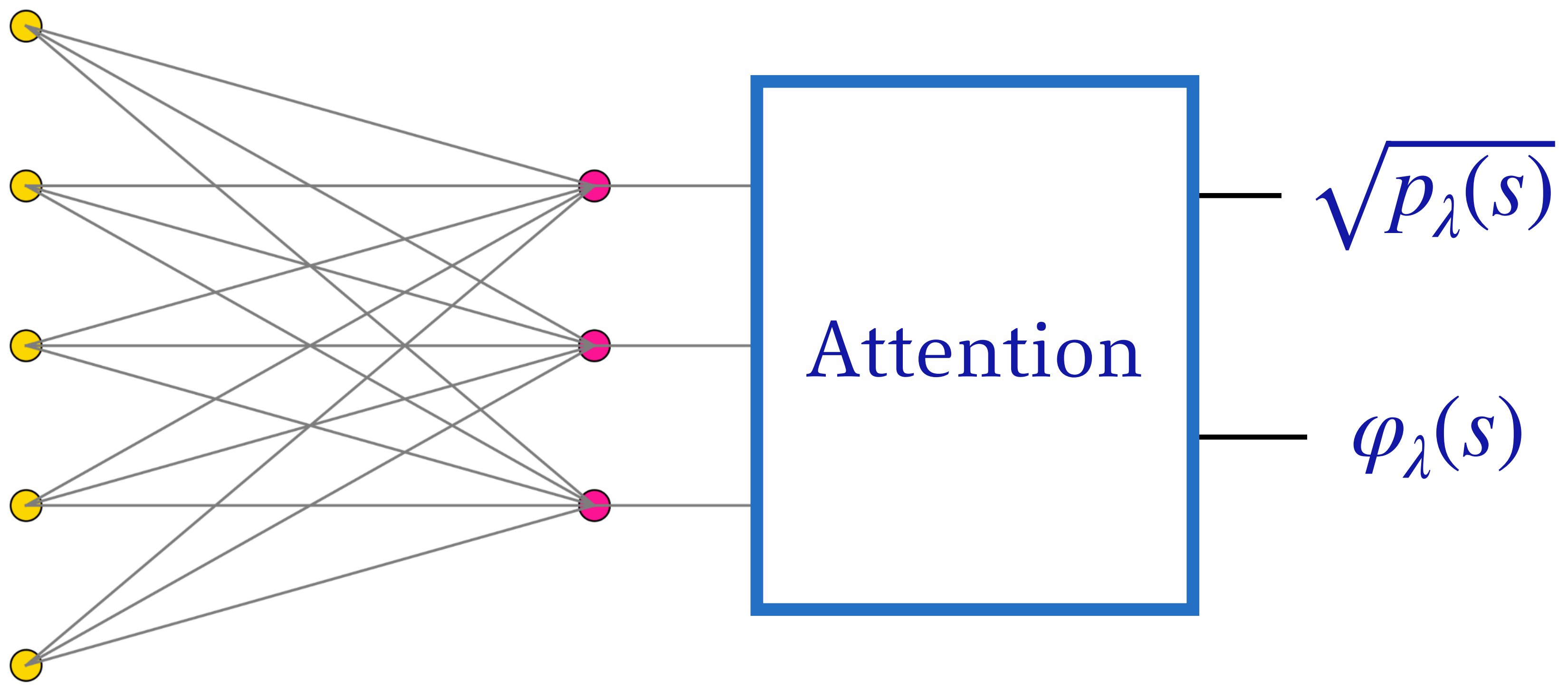
Using neural network to reduce errors

Neural shadow quantum state [Wei-Coish-Roangh-Muschik, '23]



Mixed states [arXiv:2405.06864]

Pure state $|\psi\rangle$



Mixed state $\rho = \begin{pmatrix} p_1|\psi_1\rangle\langle\psi_1| & 0 & 0 & \cdots \\ 0 & p_2|\psi_2\rangle\langle\psi_2| & 0 & \cdots \\ \vdots & \vdots & \ddots & \end{pmatrix}$

Additional qubits (B) to purity the mixed state

$$|\Psi\rangle = \sqrt{p_1}\,|\psi_1\rangle_A|0\rangle_B + \sqrt{p_2}\,|\psi_2\rangle_A|1\rangle_B + \sqrt{p_3}\,|\psi_3\rangle_A|2\rangle_B + \ldots$$

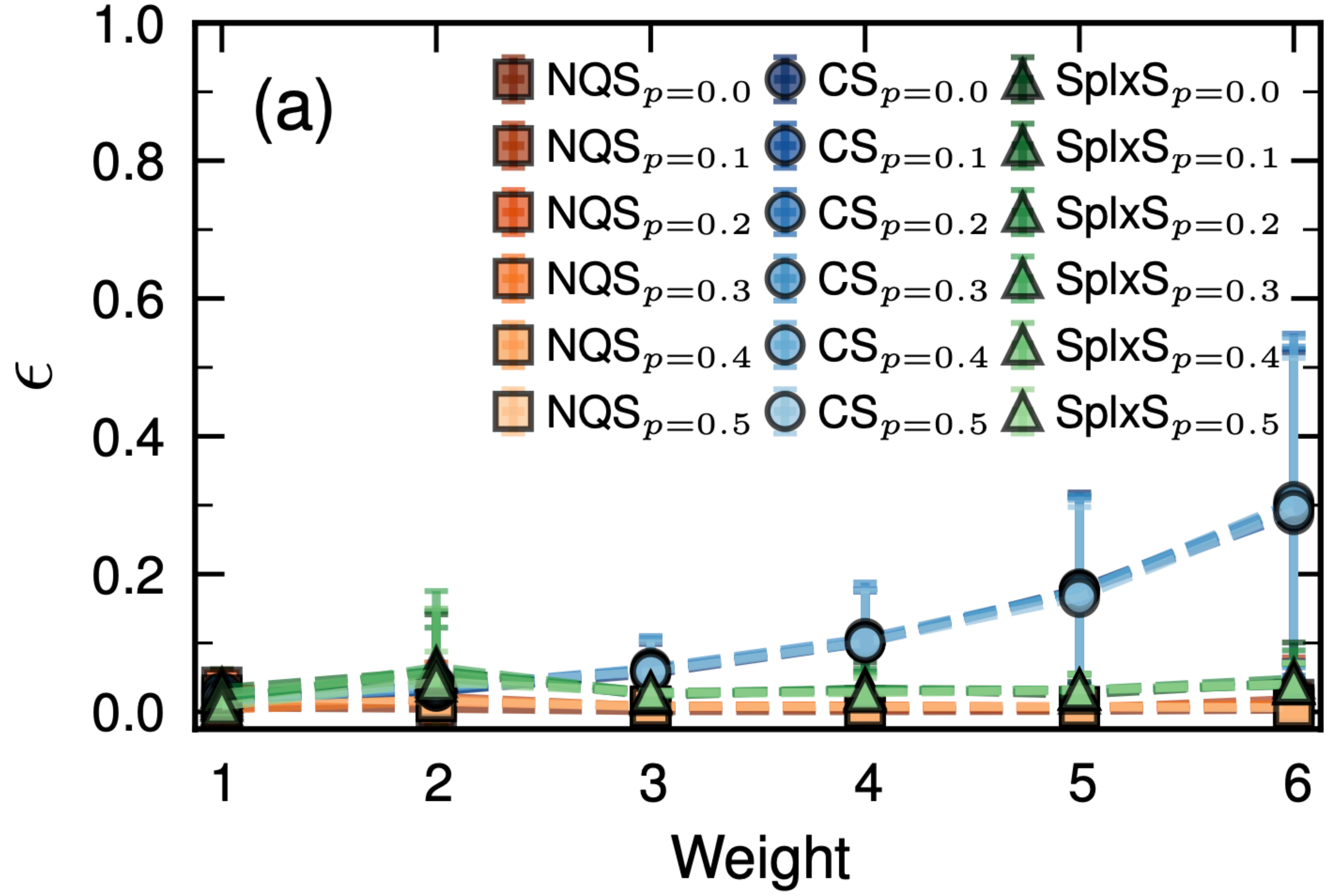
$$\rho = \mathrm{tr}_B|\Psi\rangle\langle\Psi|$$

Numerical results

6 qubit GHZ state: $|00\ldots0\rangle + |11\ldots1\rangle$

Accuracy of Pauli observable

Error

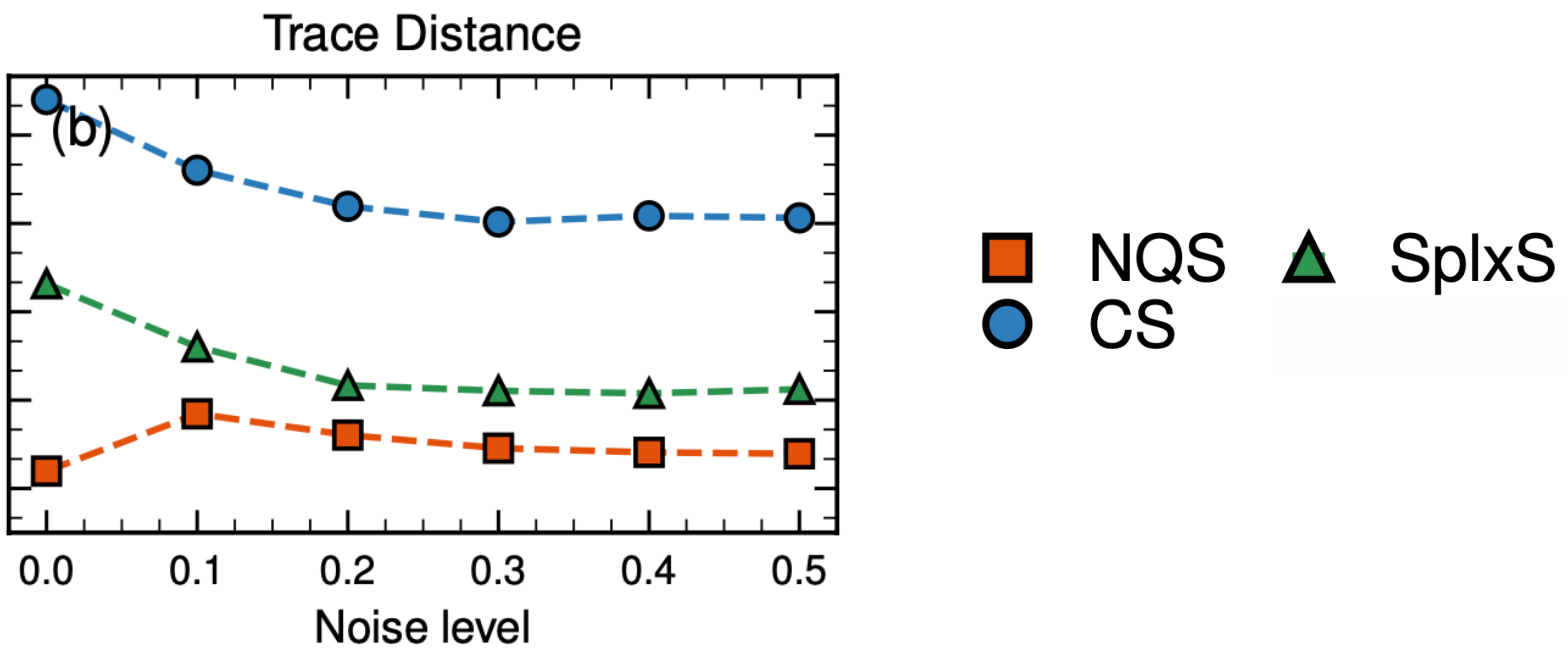


(Number of non-identity Paulis)

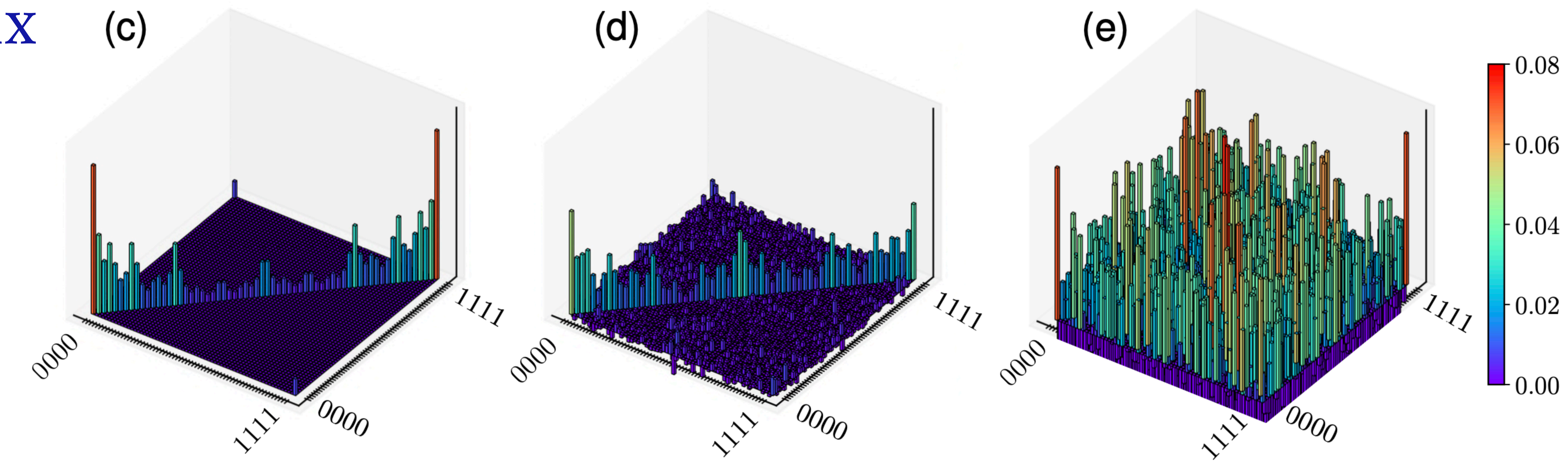
$IXIIII$: weight 1

$XXYZIY$: weight 5

Numerical results



Density matrix



Theory Neural shadow Classical shadow

Conclusion

- Reducing sampling complexity is a critical challenge in quantum computing

Even without additional experimental information,
we can still improve the accuracy of estimating physical quantities
through post-processing

Neural shadow quantum states (autoregressive model) works well
for both pure and mixed states