# Quantum ML in HEP

# Predicting many properties of a quantum system from very few measurements

New method for an approximate classical description of a quantum state called *Classical Shadow*.

- M different properties can be efficiently predicted with order(log(M)) measurements.

- The n° of measurements required respects information-theoretic lower bounds and is independent on the n° of *qubits* (system size).

- Use cases: quantum fidelities, entanglement entropies, two-point correlation functions, expectation values of local observables and the energy variance of many-bod local Hamiltonians.

# Need for Classical shadows

List of predictive tasks essential to build, calibrate and construct a quantum system.

- Exploit classical shadows to develop further quantum hardware.

- The prediction power of Quantum State Tomography and other techniques abates exponentially with the system size:

  - ➢ Number of parameters describing a quantum state exponential in $n$.

  - ➢ The knowledge of each parameter is limited by QM theory (measure identical states multiple times to get statistics).

  - ➢ All measurements are stored classically (exponential memory needed).

# Need for Classical shadows

Classical shadows combine

## Quantum State Tomography

o Can use polynomial number of samples in suitable conditions .

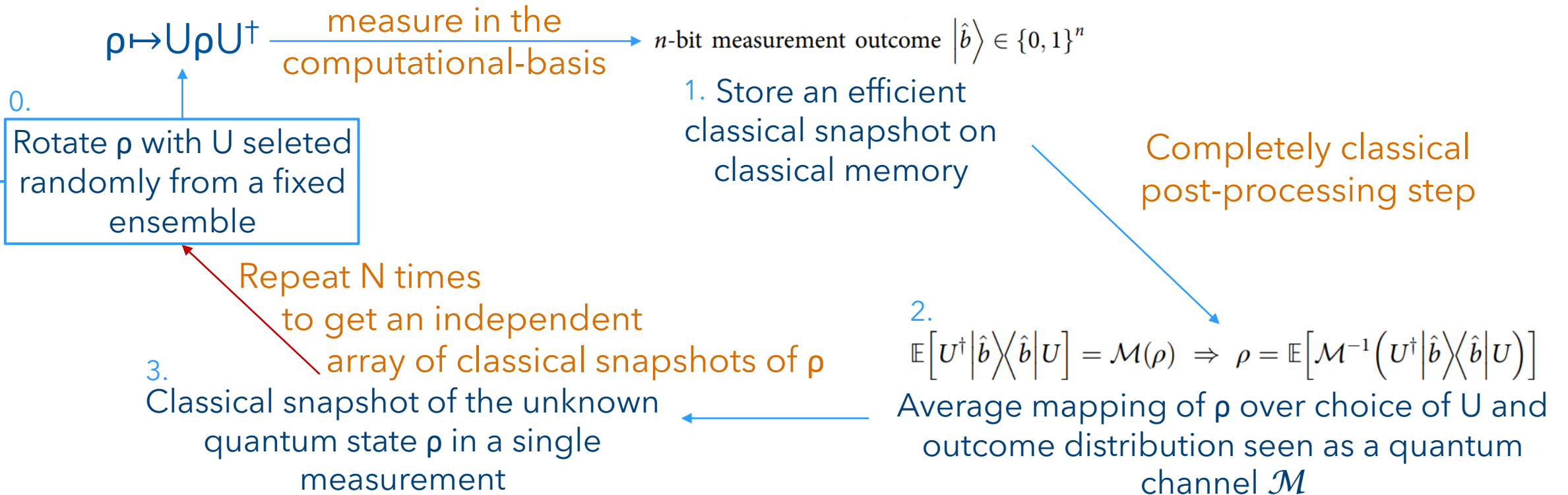o Conveys rigorous statistical convergence guarantees.

## Shadow Tomography (Aaronson formalism)

o Functions (non-)linear in ρ of the unknown state:

$$o_i(\rho) = \mathrm{trace}(O_i\rho) \quad 1 \leq i \leq M$$

o No need to fully characterize the quantum state  and polynomial n° of state copies to predict an exponential n° of $O_i$ observables.

o Exponentially long quantum circuits.

## Stabilizer Formalism (efficient implementation)

o It allows to store efficiently on a classical memory the classical shadow.

o It is a decomposition technique for local observables or global features.

# Procedure

$$\rho \mapsto U\rho U^\dagger$$

measure in the computational-basis

$n$-bit measurement outcome $\left|\hat{b}\right\rangle \in \{0,1\}^n$

0.

Rotate ρ with U seleted randomly from a fixed ensemble

1. Store an efficient classical snapshot on classical memory

Completely classical post-processing step

Repeat N times
to get an independent array of classical snapshots of ρ

2.
$$\mathbb{E}\left[U^\dagger\left|\hat{b}\right\rangle\left\langle\hat{b}\right|U\right] = \mathcal{M}(\rho) \Rightarrow \rho = \mathbb{E}\left[\mathcal{M}^{-1}\left(U^\dagger\left|\hat{b}\right\rangle\left\langle\hat{b}\right|U\right)\right]$$

3.
Classical snapshot of the unknown quantum state ρ in a single measurement

Average mapping of ρ over choice of U and outcome distribution seen as a quantum channel $\mathcal{M}$

# Classical shadow algorithm

- The classical shadow of size N is:

$$S(\rho; N) = \left\{ \hat{\rho}_1 = \mathcal{M}^{-1}\left( U_1^\dagger \left| \hat{b}_1 \right\rangle \left\langle \hat{b}_1 \right| U_1 \right), \dots, \right.$$

$$\left. \hat{\rho}_N = \mathcal{M}^{-1}\left( U_N^\dagger \left| \hat{b}_N \right\rangle \left\langle \hat{b}_N \right| U_N \right) \right\}$$

| |
|---|
| 1 **function** LINEARPREDICTIONS($O_1, \dots, O_M$, S($\rho$; N), K) |
| 2 Import S($\rho$; N) = $[\hat{\rho}_1, \dots, \hat{\rho}_N]$ ▷ Load classical shadow |
| 3 Split the shadow into K equally-sized parts and set ▷ Construct K estimators of $\rho$ |
| $\hat{\rho}_{(k)} = \frac{1}{\lfloor N/K \rfloor} \sum_{l=(k-1)\lfloor N/K \rfloor + 1}^{k\lfloor N/K \rfloor} \hat{\rho}_l$ |
| 4    **for** $i = 1$ to M **do** |
| 5 Output $\hat{o}_i(N, K) = \text{median}\left\{ \text{tr}\left( O_i \hat{\rho}_{(1)} \right), \dots, \text{tr}\left( O_i \hat{\rho}_{(K)} \right) \right\}$. ▷ Median of means estimation |

- The ensambles for random U chosen are:

  ➢ Clifford measurement  $\mathcal{M}_n^{-1}(X) = (2^n + 1)X - \mathbb{I}.$  (*n*-qubit Clifford unitaries)

  ➢ Pauli measurement  $\mathcal{M}_P^{-1} = \bigotimes_{i=1}^n \mathcal{M}_1^{-1}.$  (single-qubit Clifford unitaries, we measure each qubit in a Pauli basis)

# Performance guarantees & Information-theoretic bounds

**Theorem 1 (informal version).** *Classical shadows of size N suffice to predict M arbitrary linear target functions* $\text{tr}(O_1\rho), \dots, \text{tr}(O_M\rho)$ *up to additive error* $\epsilon$ *given that* $N \geq (\text{order}) \log(M) \max_i \|O_i\|_{\text{shadow}}^2 / \epsilon^2$. *The definition of the norm* $\|O_i\|_{\text{shadow}}$ *depends on the ensemble of unitary transformations used to create the classical shadow.*

**Theorem 2 (informal version).** *Any procedure based on single-copy measurements, that can predict any M linear functions* $\text{tr}(O_i\rho)$ *up to additive error* $\epsilon$, *requires at least* $(\text{order}) \log(M) \max_i \|O_i\|_{\text{shadow}}^2 / \epsilon^2$ *measurements.*

The two theorems states that:

- Classical shadows have a minimum number of single measurements to achieve an accurate prediction of M functions.

- This number is reached unavoidably.

# Numerical experiments

- Use of synthetic data (up to 160 qubits)
- Compare classical shadows with NNQST

The task is to learn a classical representation of an unknown quantum state and using the representation to predict various properties.

### Neural Network Quantum State Tomography

It is a generative model based on DNN trained on independent quantum measurement outcomes with local SIC\tetrahedral positive-operator valued measures (POVMs)
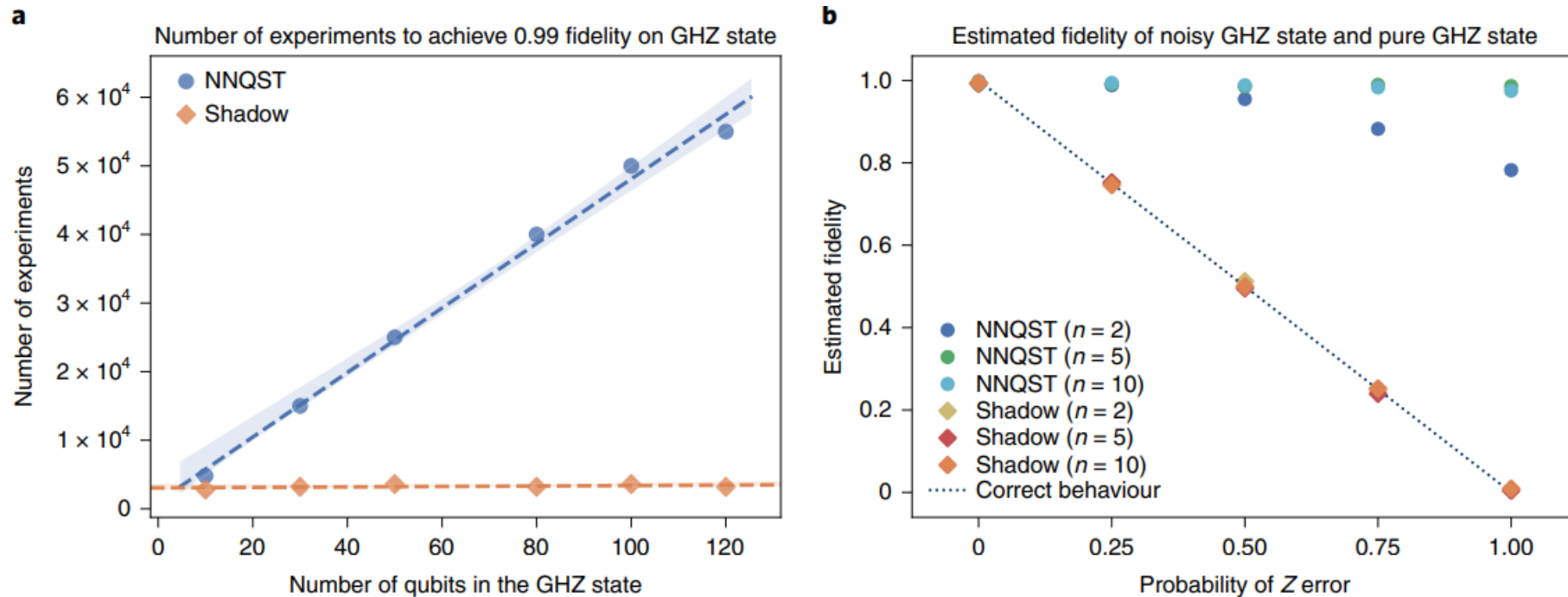
# Quantum fidelity



**a** Number of experiments to achieve 0.99 fidelity on GHZ state

**b** Estimated fidelity of noisy GHZ state and pure GHZ state

**Fig. 2 | Predicting quantum fidelities using classical shadows (Clifford measurements) and NNQST. a,** Number of measurements required to identify an $n$-qubit GHZ state with 0.99 fidelity. The shaded regions show the s.d. of the needed number of experiments over 10 independent runs. The dashed lines are the linear regression lines for the number of experiments under different system sizes. **b,** Estimated fidelity between a perfect GHZ target state and a noisy preparation, where Z errors can occur with probability $p \in [0, 1]$, under $6 \times 10^4$ experiments. The dotted line represents the true fidelity as a function of $p$. NNQST can only estimate an upper bound on quantum fidelity efficiently, so we consider this upper bound for NNQST and use quantum fidelity for the classical shadow.
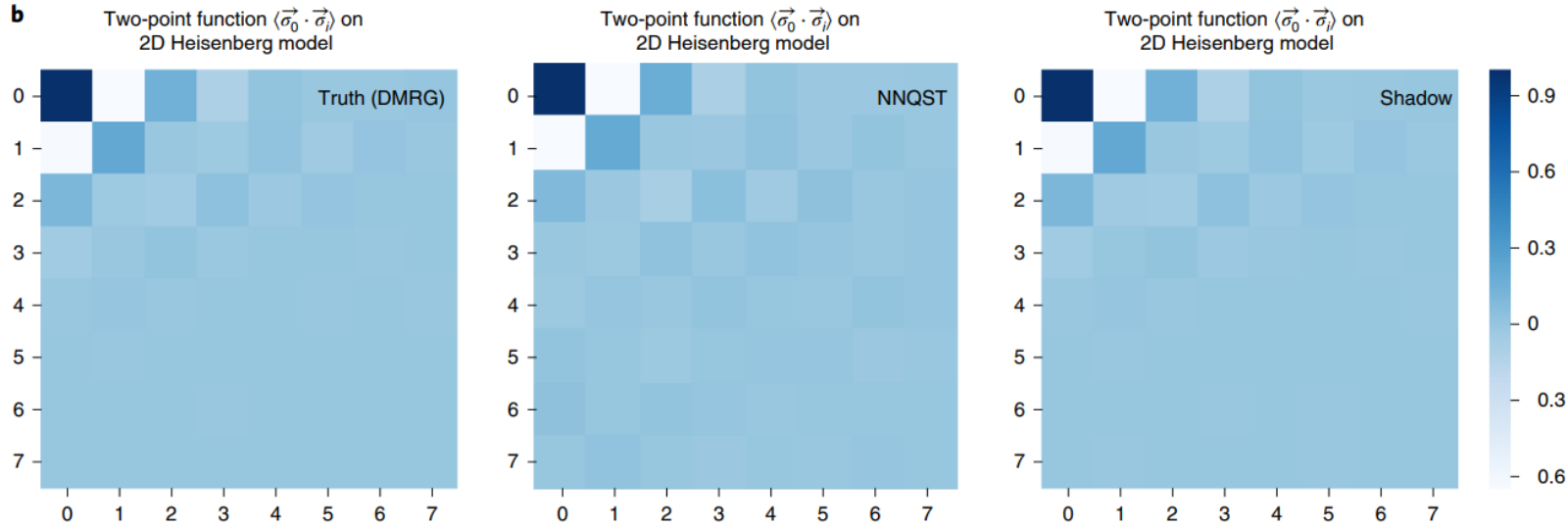
# Two-point correlation functions



**Fig. 3 | Predicting two-point correlation functions using classical shadows (Pauli measurements) and NNQST. a**, Predictions of two-point functions $\langle \sigma_0^z \sigma_i^z \rangle$ for ground states of the 1D critical antiferromagnetic TFIM with 50 lattice sites. These are based on $2^{19}$ random Pauli measurements. **b**, Predictions of two-point functions $\langle \vec{\sigma}_0 \cdot \vec{\sigma}_i \rangle$ for the ground state of the 2D antiferromagnetic Heisenberg model with $8 \times 8$ lattice sites. The predictions are based on $2^{19}$ random Pauli measurements. **c**, Classical processing time (CPU time in seconds) and prediction error (the largest among all pairs of two-point correlations) over different numbers of measurements: $\{2^{11}, ..., 2^{19}\}$. The quantum measurement scheme in classical shadows (Pauli) is the same as the POVM-based neural network tomography (NNQST) in ref. [3]. The only difference is the classical post-processing. As the number of measurements increases, the processing time increases, while the prediction error decreases.
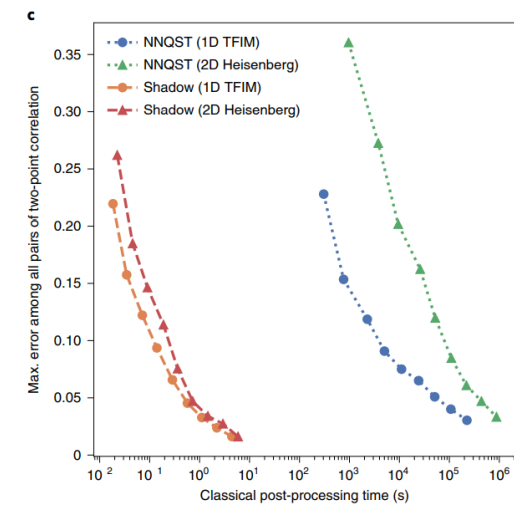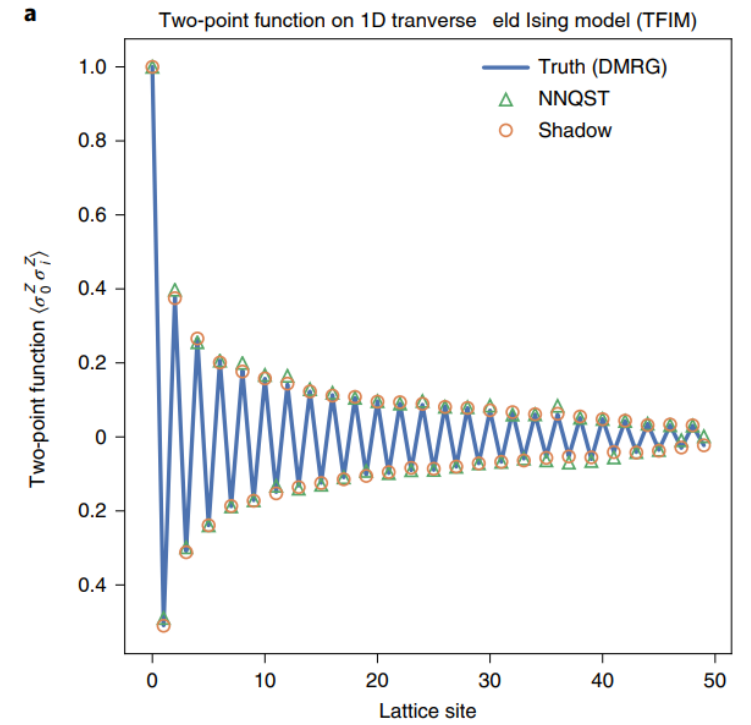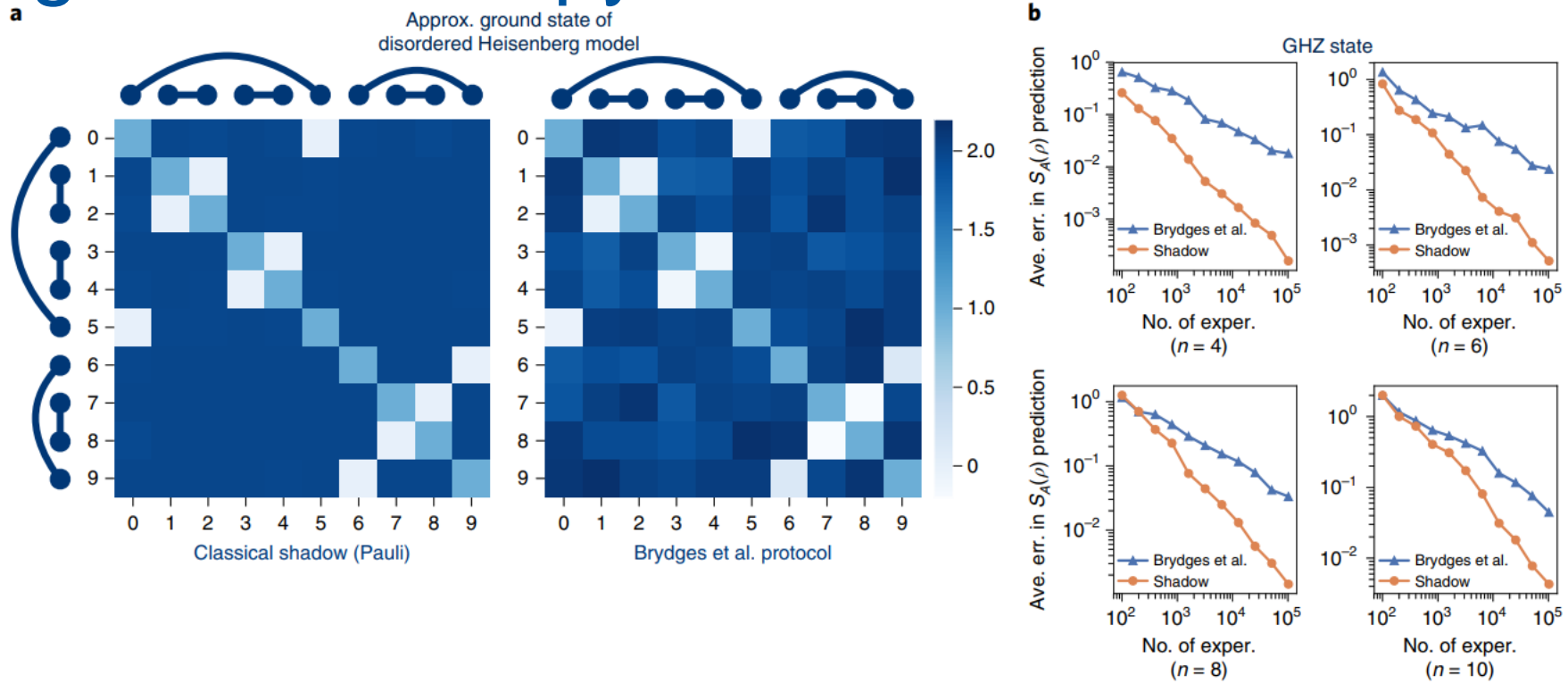
# Entanglement entropy



**Fig. 4 | Predicting entanglement Rényi entropies using classical shadows (Pauli measurements) and the Brydges et al. protocol. a,** Prediction of second-order Rényi entanglement entropy for all subsystems of size at most two in the approximate ground state of a disordered Heisenberg spin chain with 10 sites and open boundary conditions. The classical shadow is constructed from 2,500 quantum measurements. The predicted values using the classical shadow visually match the true values with a maximum prediction error of 0.052. The Brydges et al. protocol[20] results in a maximum prediction error of 0.24. **b,** Comparison of classical shadows and the Brydges et al. protocol[20] for estimating second-order Rényi entanglement entropy in GHZ states. We consider the entanglement entropy of the subsystem with size $n/2$ on the left side.
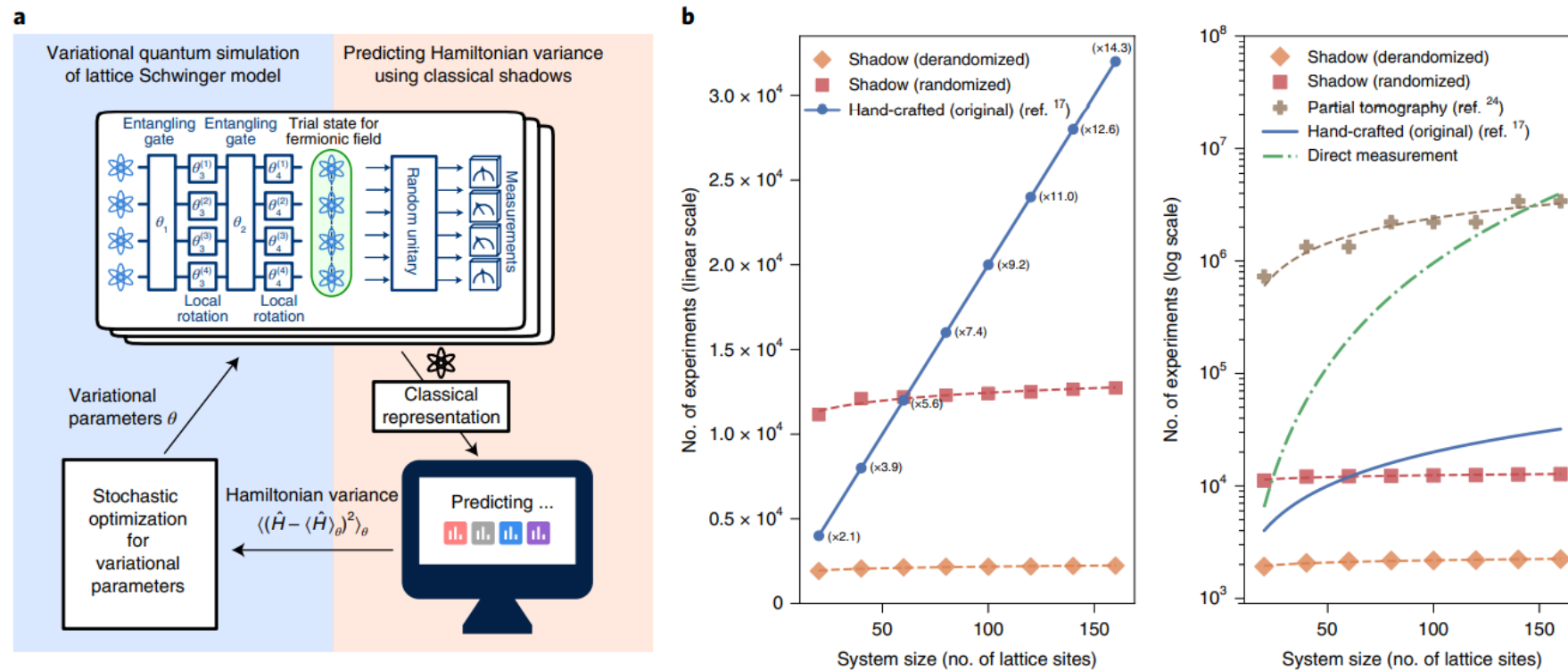
# Lattice Schwinger model



**Fig. 5 | Application of classical shadows (Pauli measurements) to variational quantum simulation of the lattice Schwinger model. a,** An illustration of variational quantum simulation and the role of classical shadows. **b,** Comparison between different approaches in the number of measurements needed to predict all 4-local Pauli observables in the expansion of $\langle(\hat{H} - \langle\hat{H}\rangle_\theta)^2\rangle_\theta$ with an error equivalent to measuring each Pauli observable at least 100 times. We include a linear-scale plot that compares classical shadows with the original hand-designed measurement scheme in ref. [18] (left) and a log-scale plot that compares with other approaches (right). In the linear-scale plot, (×T) indicates that the original scheme uses T times the number of measurements compared to classical shadows (derandomized).

# Conclusions

- Classical shadows use relatively small n° of state copies to gain a classical description af a quantum state.

- Pauli measurement can be implemented efficiently on actual quantum hardwares to predict many properties of the system.

- New method allowing classical machine learning to be used for many-body physics and other applications.

# CERN Quantum Technology Initiative

## Accelerating Quantum Technology Research and Applications

# Thanks!

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