

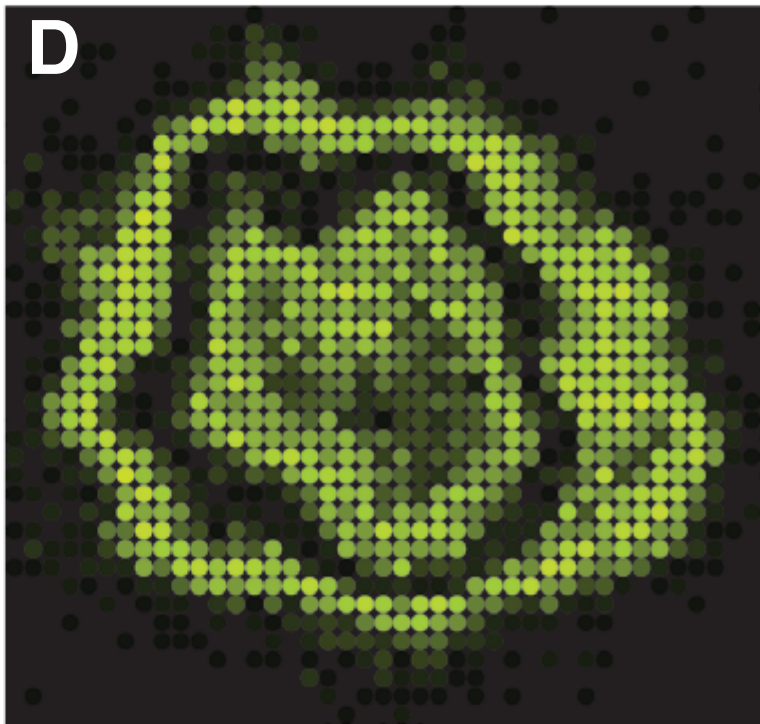
Generative Modeling of Quantum Simulators

Giacomo Torlai

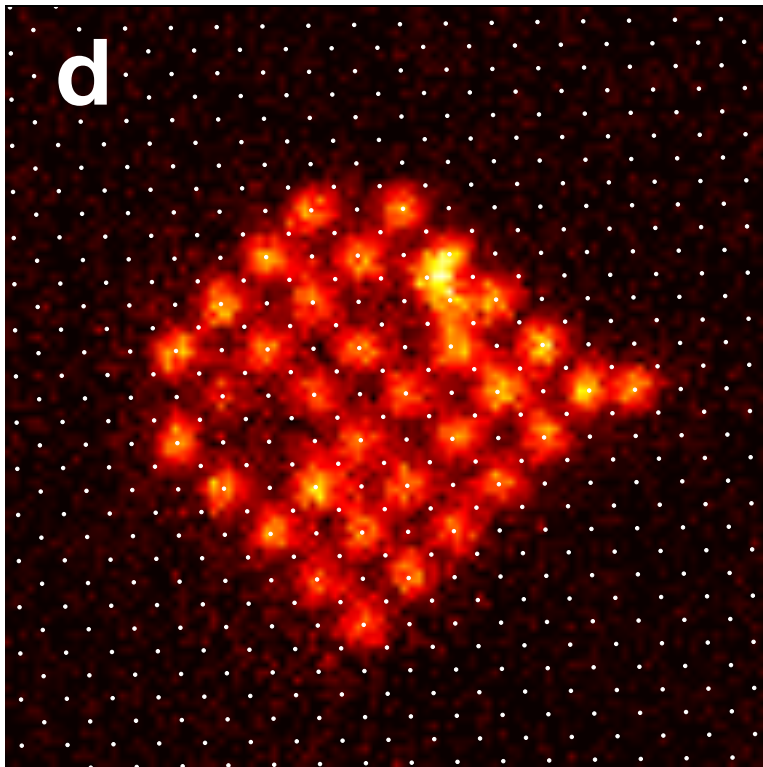
Machine Learning Quantum Matter Data
Flatiron Institute
January 23rd 2020

Quantum data

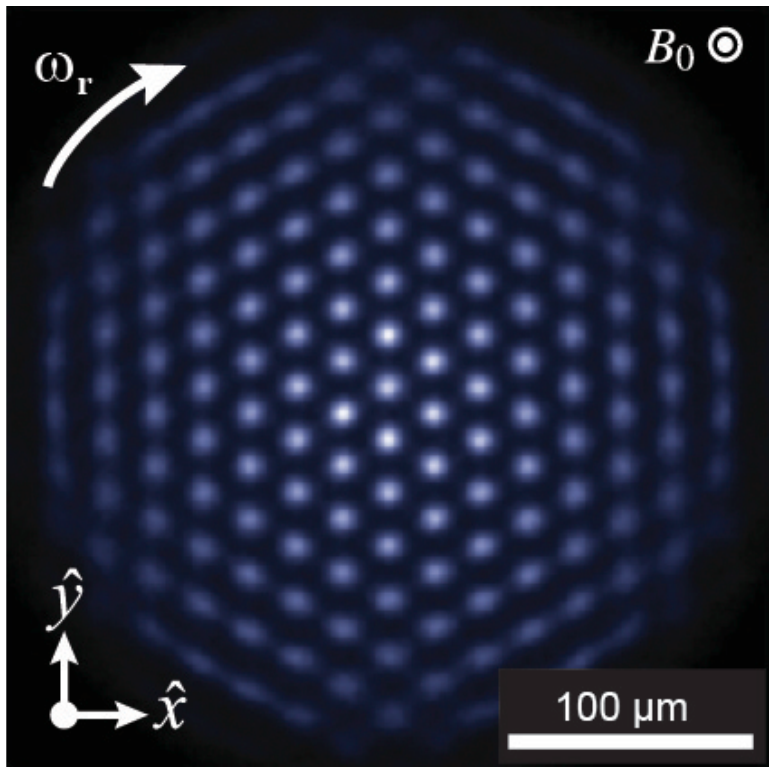
Experiments



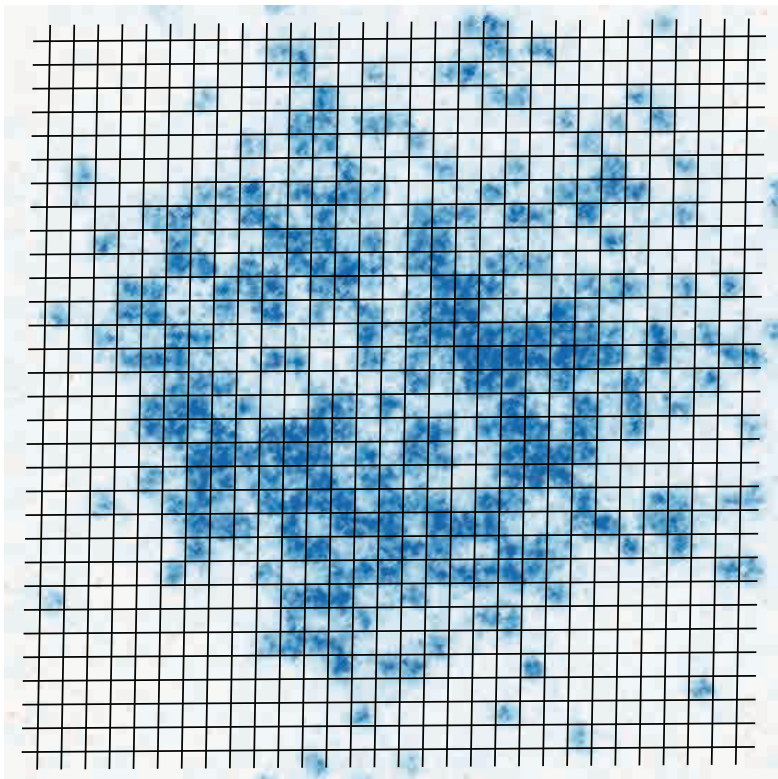
Bakr *et al*, Science (2010)



Weitenberg *et al*, Nature (2011)

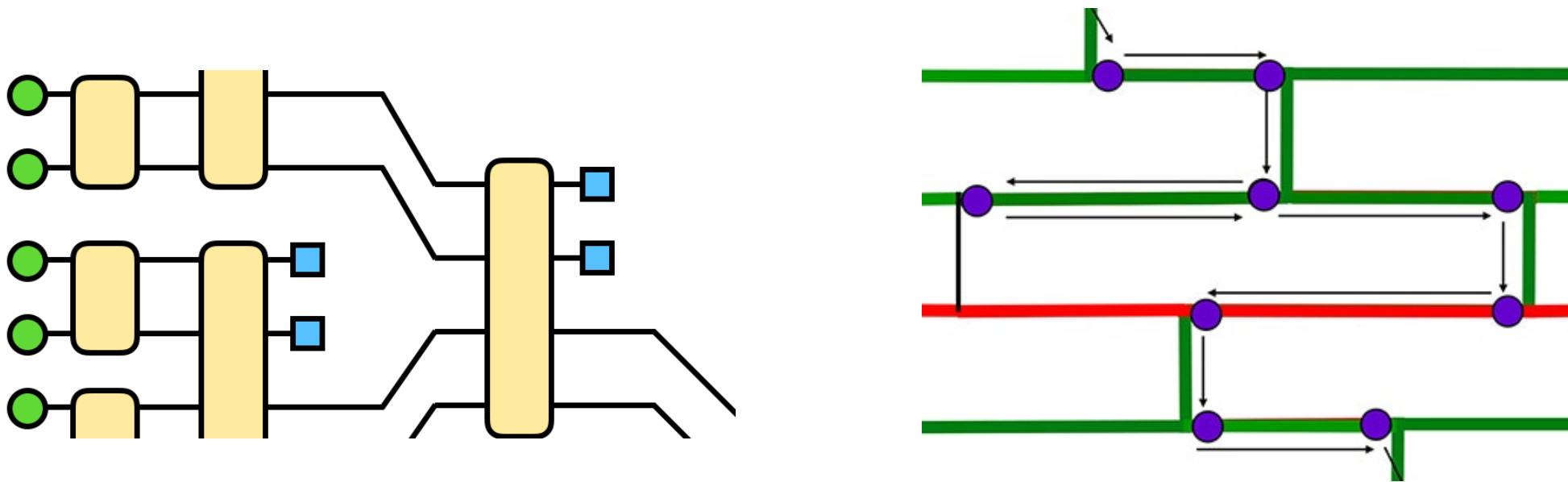


Britton *et al*, Nature (2012)

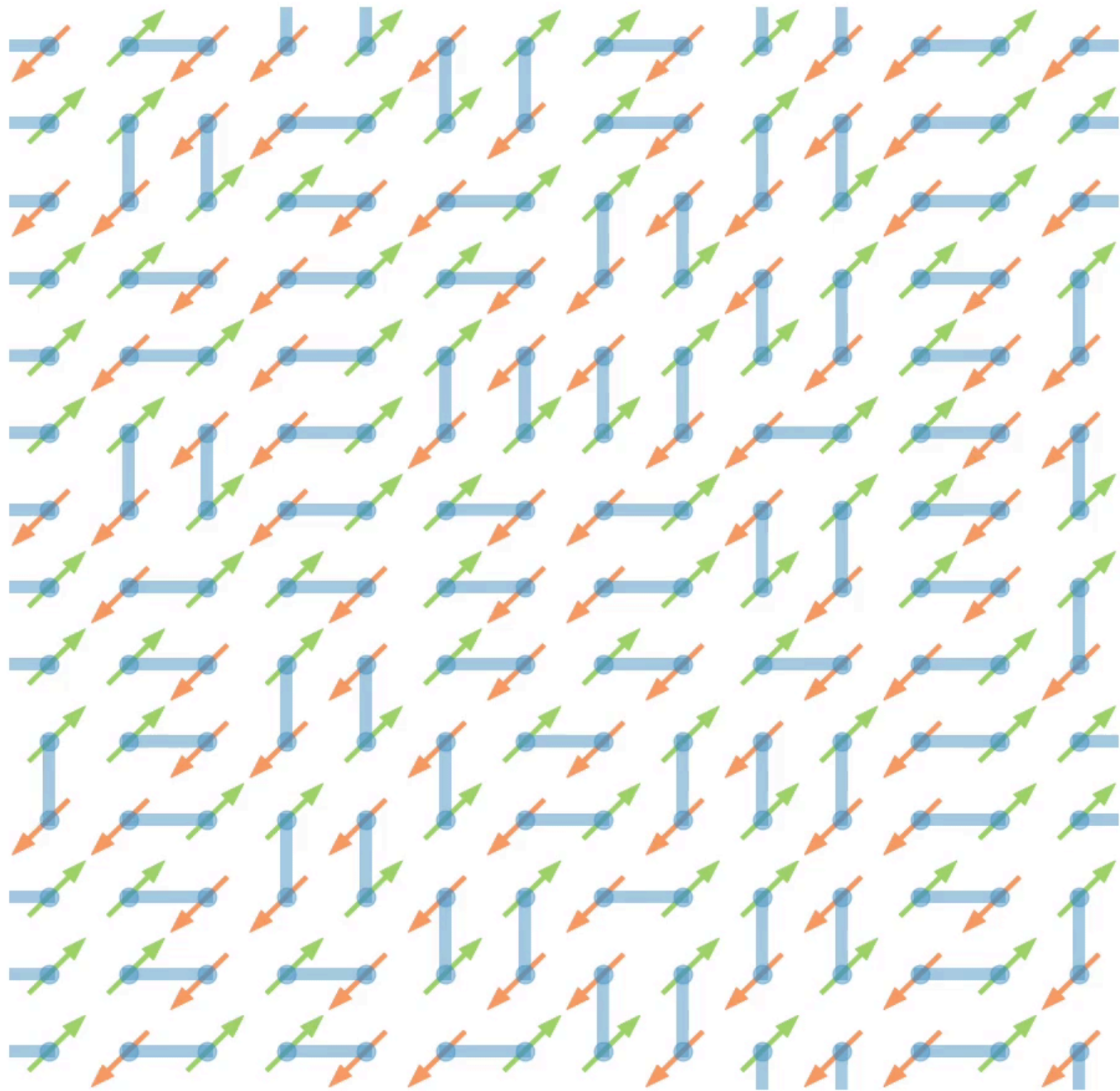


Grief *et al*, Science (2016)

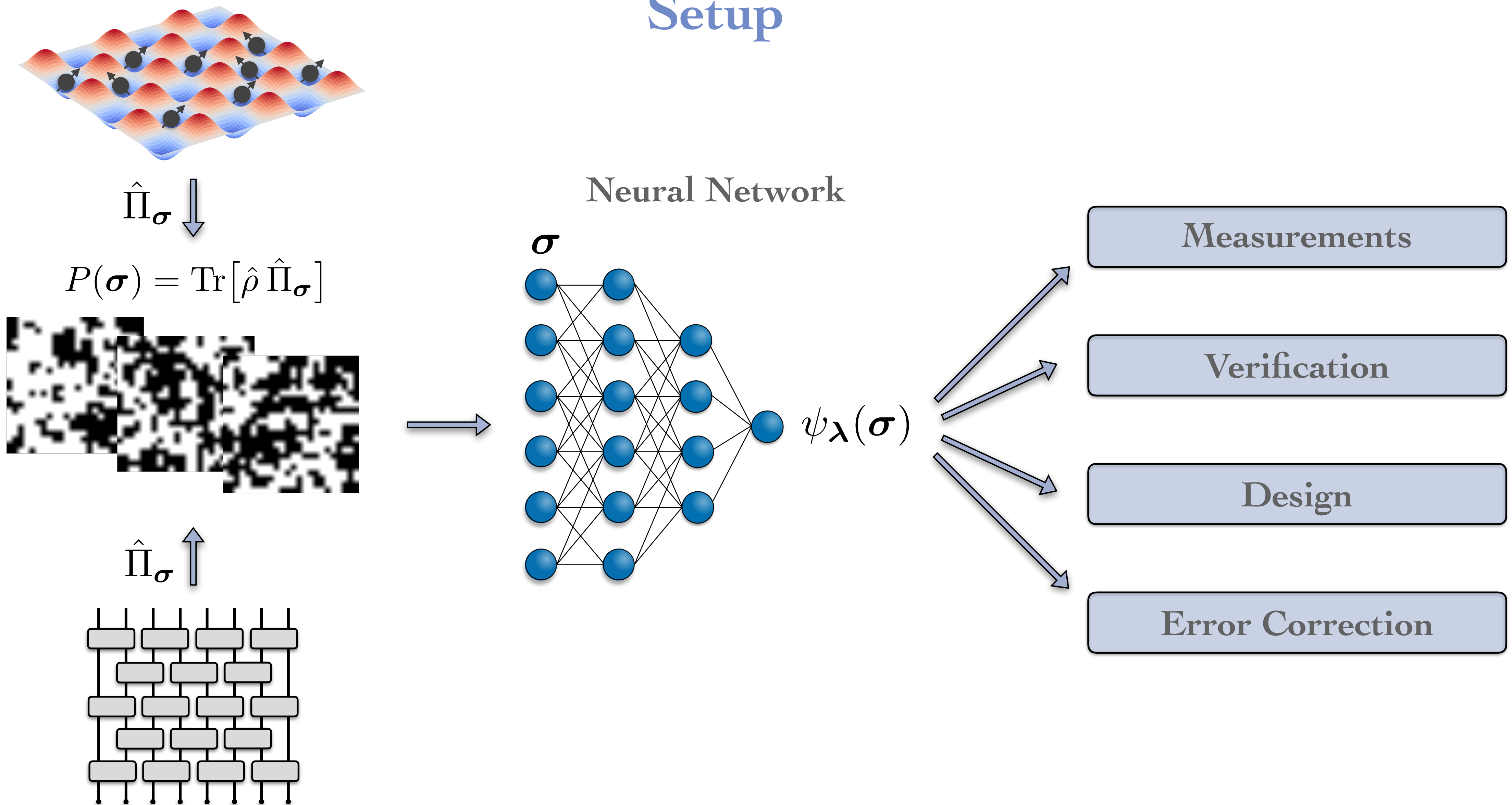
Synthetic



RVB Wavefunction



Setup



Cold Rydberg-Atom Quantum Simulator

arXiv:1904.08441 (PRL 123, 230504)

Theory

Evert van Nieuwenburg (Caltech)
Roger Melko (Perimeter Institute)
Brian Timar (Caltech)

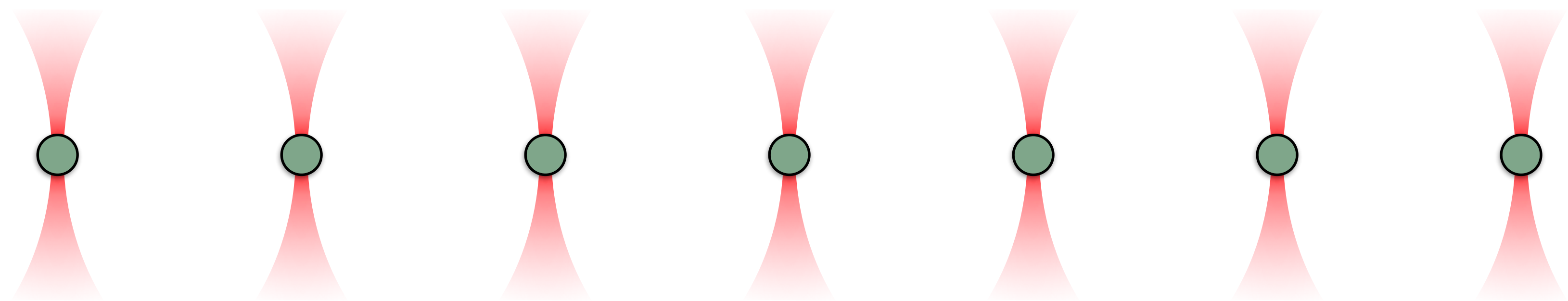
Experiment

Hannes Bernien (Chicago)
Manuel Endres (Caltech)
Markus Greiner (Harvard)
Alexander Keesling (Harvard)
Harry Levin (Harvard)
Misha Lukin (Harvard)
Ahmed Omran (Harvard)
Vladan Vuletić (MIT)

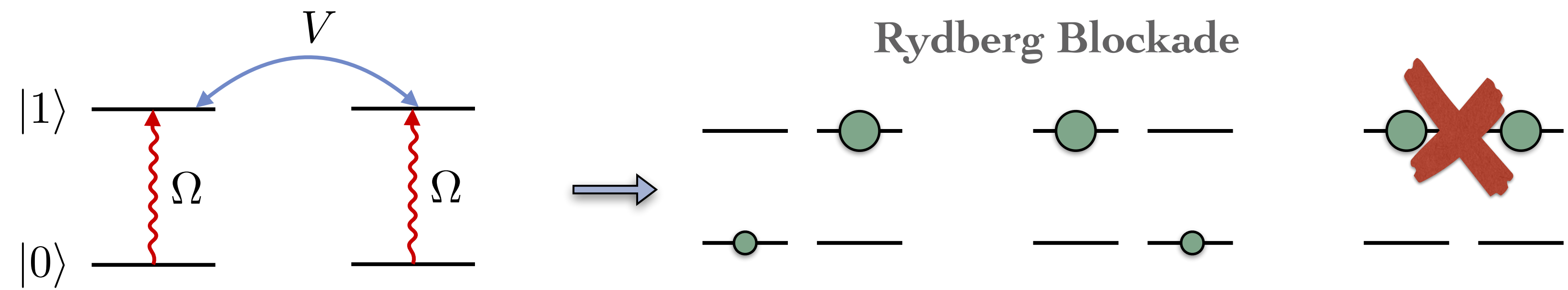
Cold neutral atoms in optical tweezers

Cold Rubidium atoms trapped by tightly-focussed laser beams.

Defect-free arrays by imaging and removing empty traps.



Drive to highly excited Rydberg states (long lifetime)



For Rydberg state $n=100$:

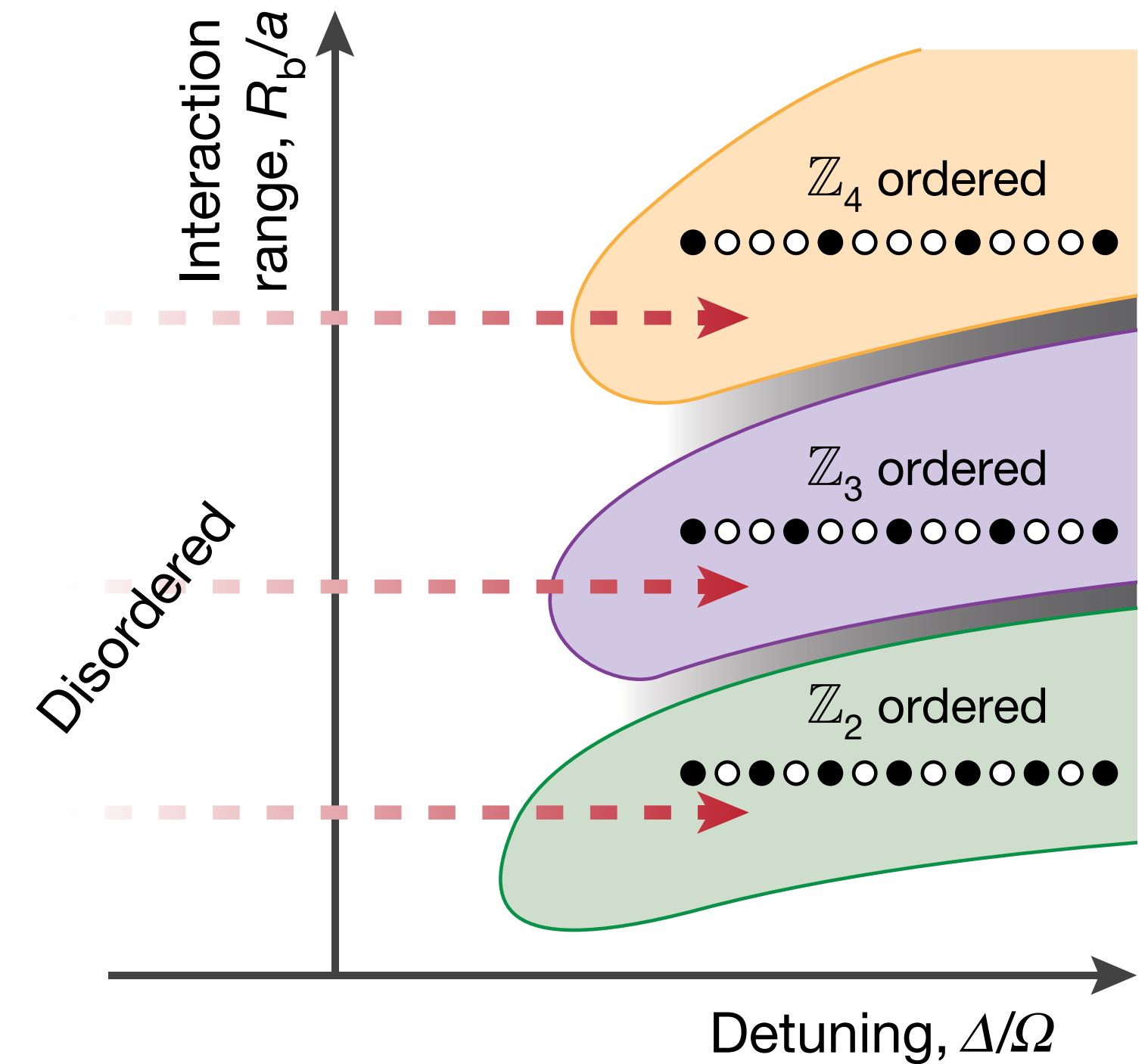
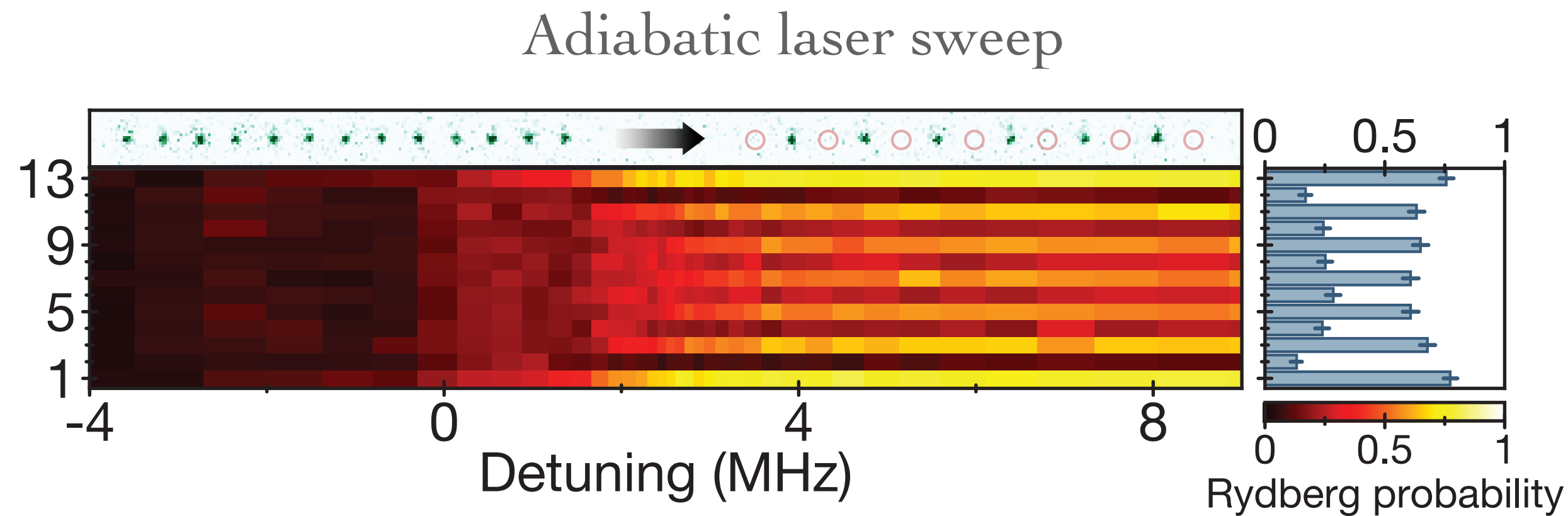
$$R_b \approx 10\mu m$$

$$V_r \approx 10^{14}V_g$$

Rydberg-atom quantum simulator

Rydberg Hamiltonian: $\hat{H}(\Omega, \Delta) = -\Delta \sum_i \hat{n}_i - \frac{\Omega}{2} \sum_i \hat{\sigma}_i^x + \sum_{i < j} V_{i,j} \hat{n}_i \hat{n}_j$

Nearest-neighbour Rydberg blockade: $n_i n_{i+1} = 0$



Ground state wavefunction: $|\Psi\rangle = \sum_{\sigma} \Psi(\sigma) |\sigma\rangle \quad \{|\sigma\rangle\} \equiv \{|n\rangle\}$

Perron-Frobenius: $\Psi(\sigma) \geq 0 \forall |\sigma\rangle \implies \{|\sigma\rangle\}$ informationally complete

$\implies P(\sigma) = |\Psi(\sigma)|^2$ uniquely identifies the ground state wavefunction

Quantum reconstruction

Set of projective measurement data $\mathcal{D} = \{\boldsymbol{\sigma}\}$ with distribution $P(\boldsymbol{\sigma}) = |\Psi(\boldsymbol{\sigma})|^2$

Generative modeling with RBMs:

$$|\psi_{\lambda}\rangle = \sum_{\boldsymbol{\sigma}} \sqrt{p_{\lambda}(\boldsymbol{\sigma})} |\boldsymbol{\sigma}\rangle \quad p_{\lambda}(\boldsymbol{\sigma}) \propto \sum_{\mathbf{h}} e^{-E_{\lambda}(\boldsymbol{\sigma}, \mathbf{h})}$$

Training by optimizing the statistical divergence:

$$\mathcal{C}_{KL}(P \parallel p_{\lambda}) = \sum_{\boldsymbol{\sigma}} P(\boldsymbol{\sigma}) \log \frac{P(\boldsymbol{\sigma})}{p_{\lambda}(\boldsymbol{\sigma})} \simeq \mathcal{L}_{\lambda} = - \sum_{\boldsymbol{\sigma} \in \mathcal{D}} \log p_{\lambda}(\boldsymbol{\sigma})$$

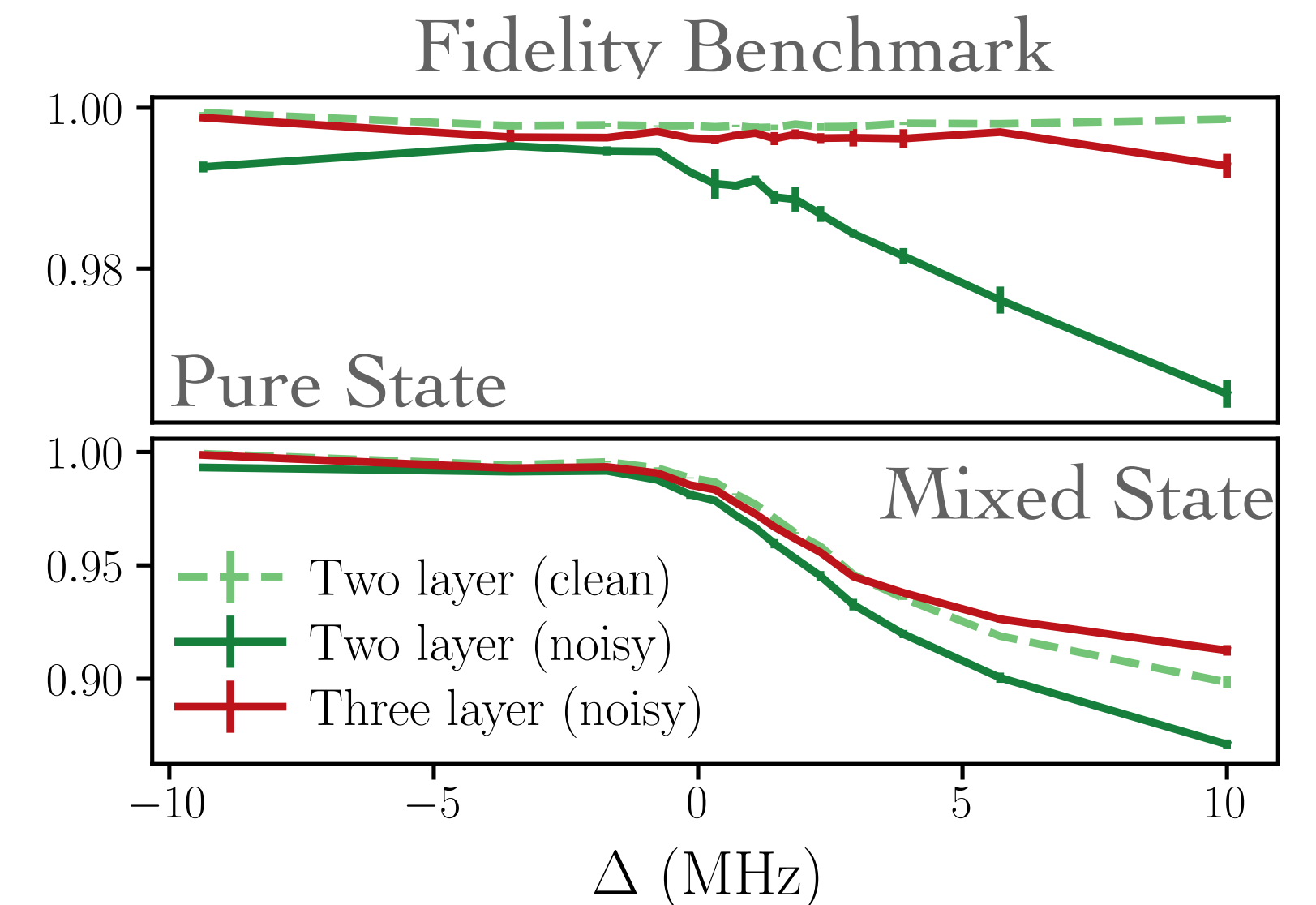
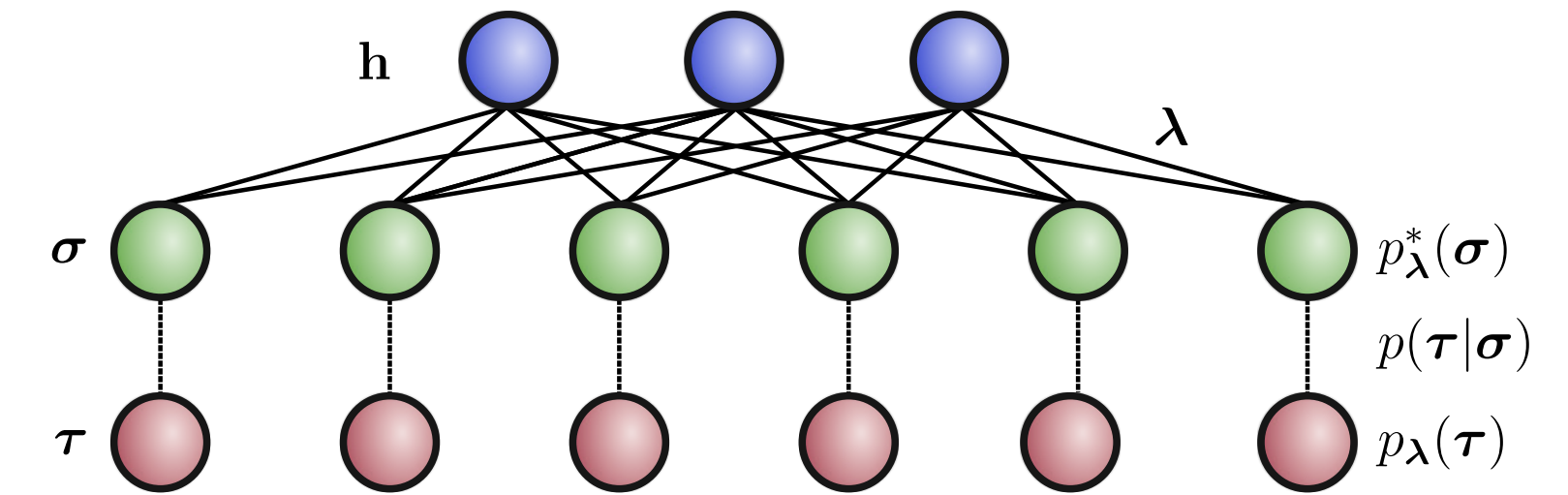
Noise-layer regularization

Readout measurement error rates are known: $p(0 \mid 1) = 0.04$, $p(1 \mid 0) = 0.01$

Modified network architecture to mitigate measurement noise:

- $\mathbf{h}$ Hidden neurons
- $\boldsymbol{\sigma}$ De-noised neurons
- $\boldsymbol{\tau}$ Visible (noisy) neurons

Noise-layer distribution: $p_{\lambda}(\boldsymbol{\tau}) = \sum_{\boldsymbol{\sigma}} p(\boldsymbol{\tau} \mid \boldsymbol{\sigma}) p_{\lambda}^*(\boldsymbol{\sigma})$



8-atom experiment

Rydberg Hamiltonian: $\hat{H}(\Omega, \Delta) = -\Delta \sum_i \hat{n}_i - \frac{\Omega}{2} \sum_i \hat{\sigma}_i^x + \sum_{i < j} \frac{V}{|i - j|^6} \hat{n}_i \hat{n}_j$

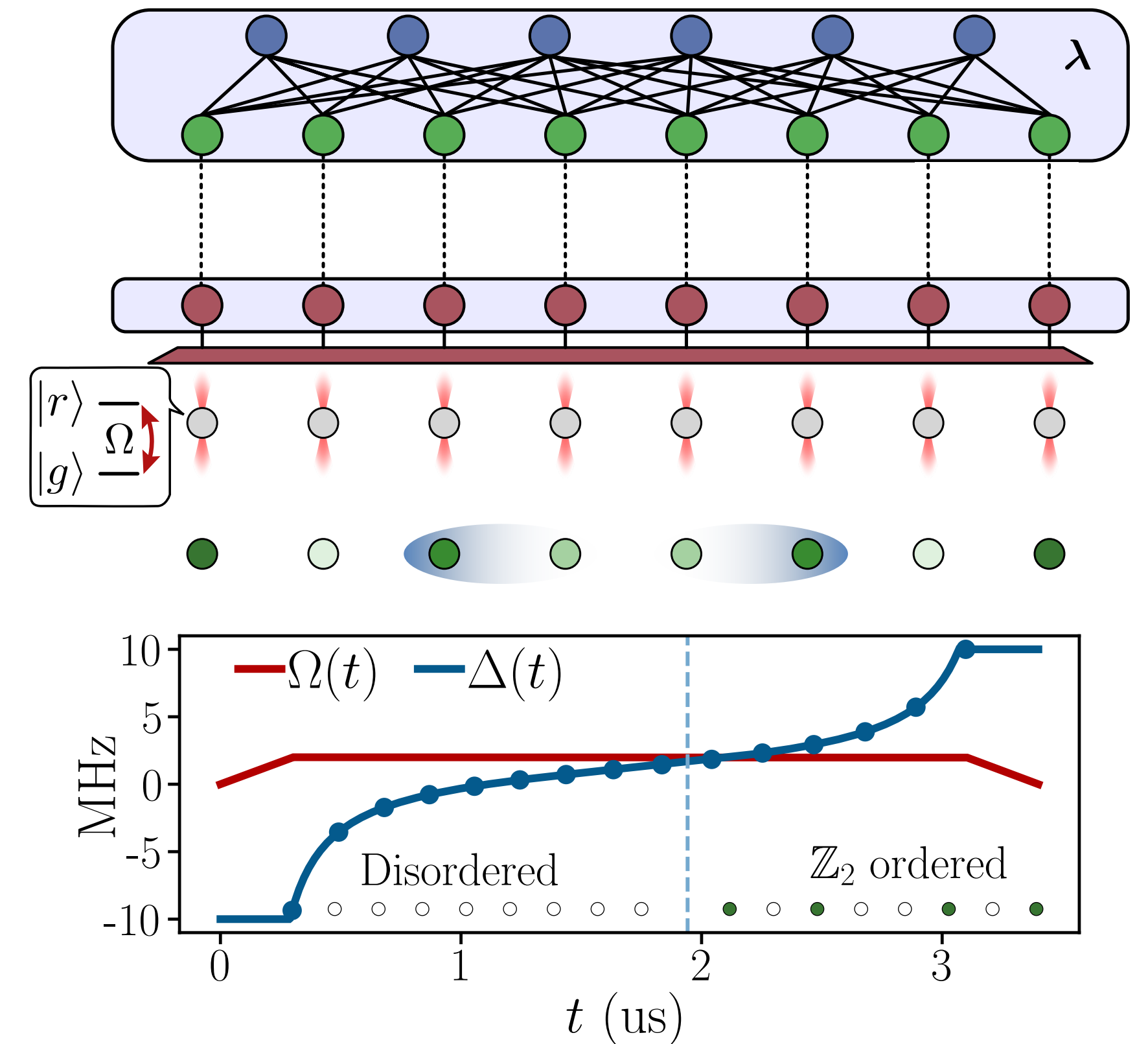
Negative detuning $\Delta < 0$: $|\Psi\rangle = |00000000\rangle$

In the Rydberg blockade regime ($\Delta > 0, V_{nn} \gg \Delta$), classical limit:

4-excitation degenerate states $\begin{cases} |10100101\rangle \\ |10010101\rangle \\ |10101001\rangle \end{cases}$

Transverse-field $\Omega \neq 0$ lifts degeneracy:

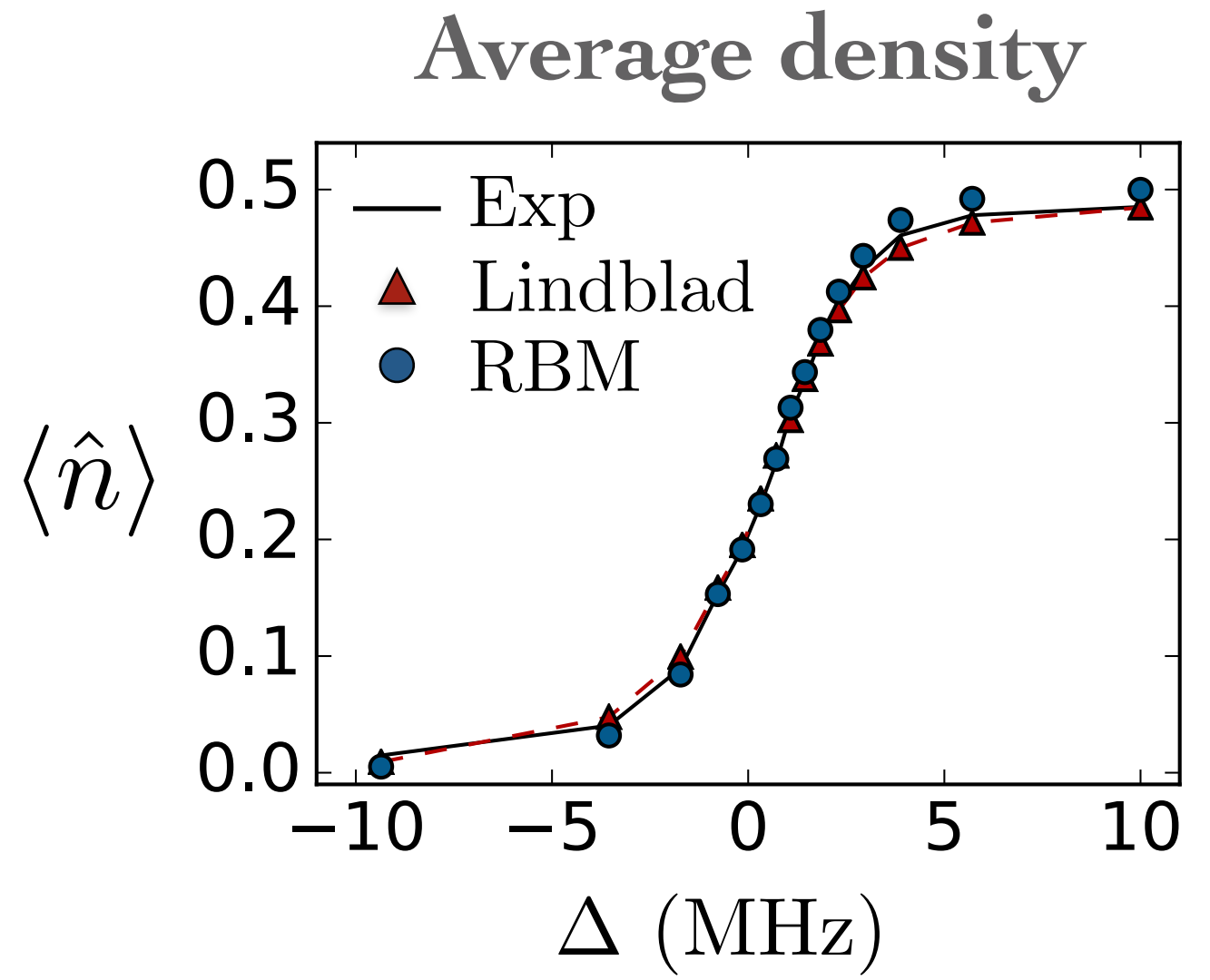
$$|\Psi_f\rangle = \frac{1}{\sqrt{2}}|10100101\rangle + \frac{1}{2}|10101001\rangle + \frac{1}{2}|10010101\rangle$$



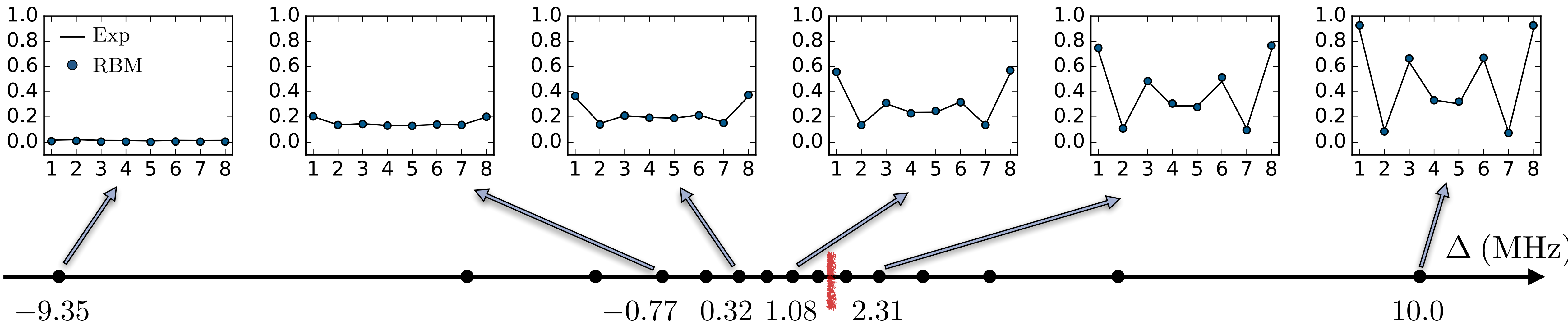
Neural-network measurements

Diagonal observables

$$\begin{aligned}\langle \hat{O} \rangle &= \langle \psi_{\lambda} | \hat{O} | \psi_{\lambda} \rangle = \sum_{\sigma} p_{\lambda}(\sigma) \mathcal{O}_{\sigma\sigma} \\ &= \frac{1}{n_{mc}} \sum_{k=1}^{n_{mc}} \mathcal{O}_{\sigma_k \sigma_k} \quad \{ \sigma_k \} \leftarrow p_{\lambda}(\sigma)\end{aligned}$$



Rydberg excitation density



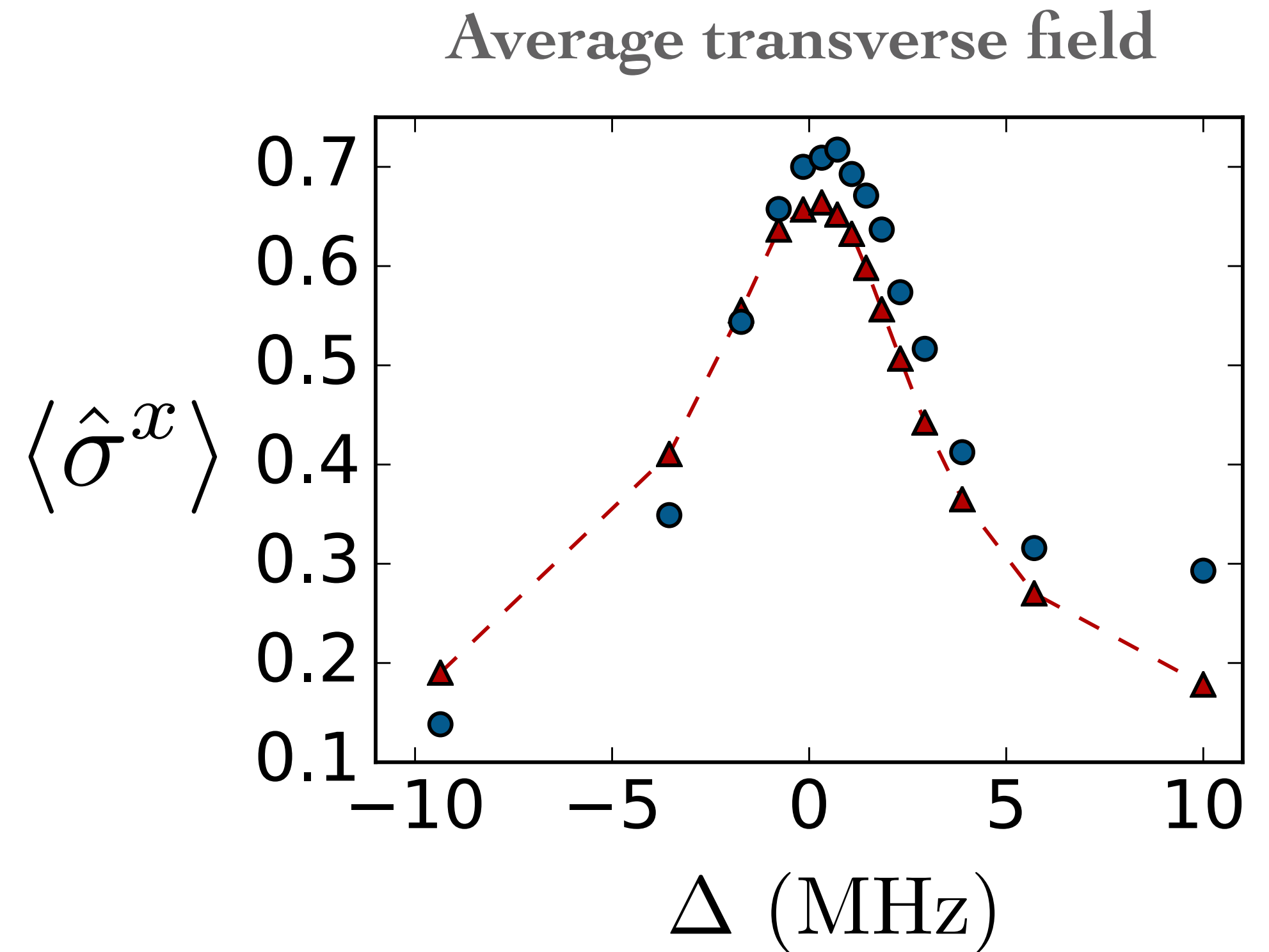
Neural-network measurements

Off-diagonal observables

$$\begin{aligned}\langle \hat{\mathcal{O}} \rangle &= \langle \psi_{\lambda} | \hat{\mathcal{O}} | \psi_{\lambda} \rangle = \sum_{\sigma, \sigma'} \sqrt{p_{\lambda}(\sigma)} \sqrt{p_{\lambda}(\sigma')} \mathcal{O}_{\sigma \sigma'} \\ &= \sum_{\sigma} p_{\lambda}(\sigma) \sum_{\sigma'} \sqrt{\frac{p_{\lambda}(\sigma')}{p_{\lambda}(\sigma)}} \mathcal{O}_{\sigma \sigma'} \\ &= \frac{1}{n_{mc}} \sum_{k=1}^{n_{mc}} \mathcal{O}^L(\sigma_k) \quad \{\sigma_k\} \leftarrow p_{\lambda}(\sigma)\end{aligned}$$

Average transverse field:

$$\begin{aligned}\mathcal{O}^L(\sigma_k) &= \frac{1}{N} \sum_{j=1}^N \sum_{\sigma'} \sqrt{\frac{p_{\lambda}(\sigma')}{p_{\lambda}(\sigma)}} \langle \sigma | \hat{\sigma}_j^x | \sigma' \rangle \\ &= \frac{1}{N} \sum_{j=1}^N \sqrt{\frac{p_{\lambda}(\sigma_1, \dots, -\sigma_j, \dots, \sigma_N)}{p_{\lambda}(\sigma_1, \dots, \sigma_j, \dots, \sigma_N)}}\end{aligned}$$



Neural-network measurements

Entanglement entropy

Second Renyi entanglement entropy:

$$\begin{aligned} S_2(\hat{\rho}_\ell) &= -\log(\text{Tr}(\hat{\rho}_\ell^2)) \\ &= \log \left[\langle \Psi_1, \Psi_2 | \text{Swap}_\ell | \Psi_1, \Psi_2 \rangle \right] \end{aligned}$$

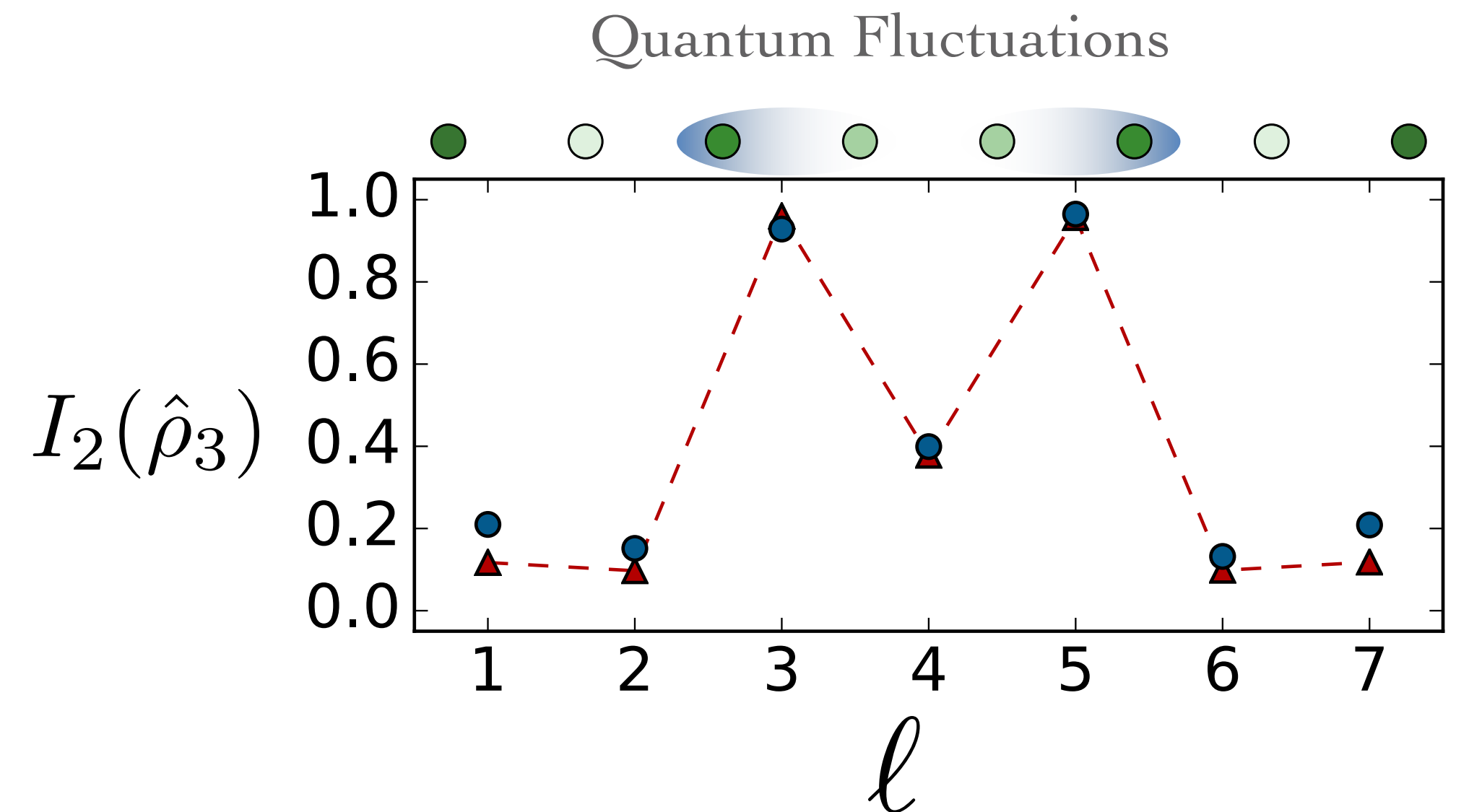
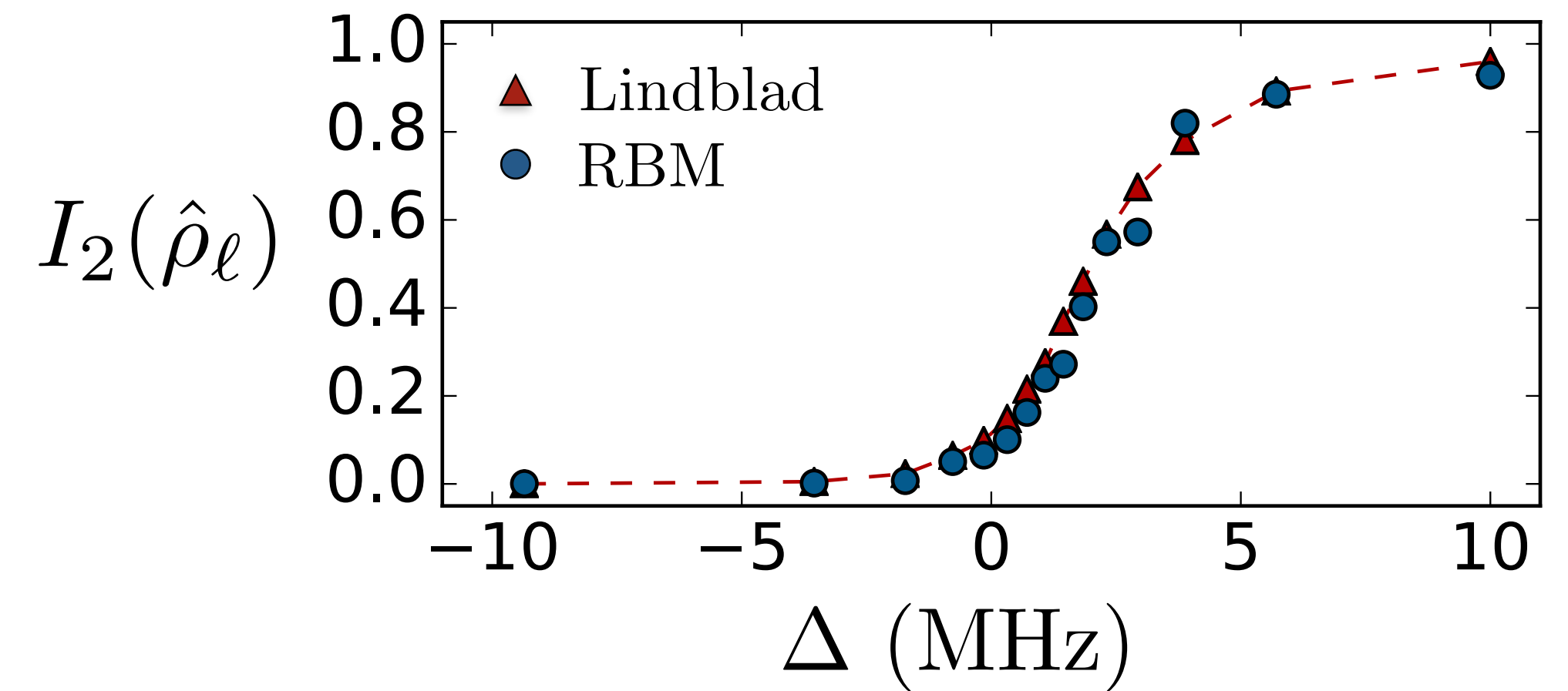
where $\hat{\rho}_\ell = \text{Tr}_{N-\ell}(|\Psi\rangle\langle\Psi|)$

Note: for $\Phi(\sigma) = \Psi(\sigma)e^{i\theta(\sigma)}$

$$S_2(\text{Tr}_{N-\ell}(|\Psi\rangle\langle\Psi|)) \geq S_2(\text{Tr}_{N-\ell}(|\Phi\rangle\langle\Phi|))$$

Wavefunctions in the Z2 phase:

$$|\Psi_f\rangle = \frac{1}{\sqrt{2}}|10100101\rangle + \frac{1}{2}|10101001\rangle + \frac{1}{2}|10010101\rangle$$



Digital Simulation of Quantum Chemistry

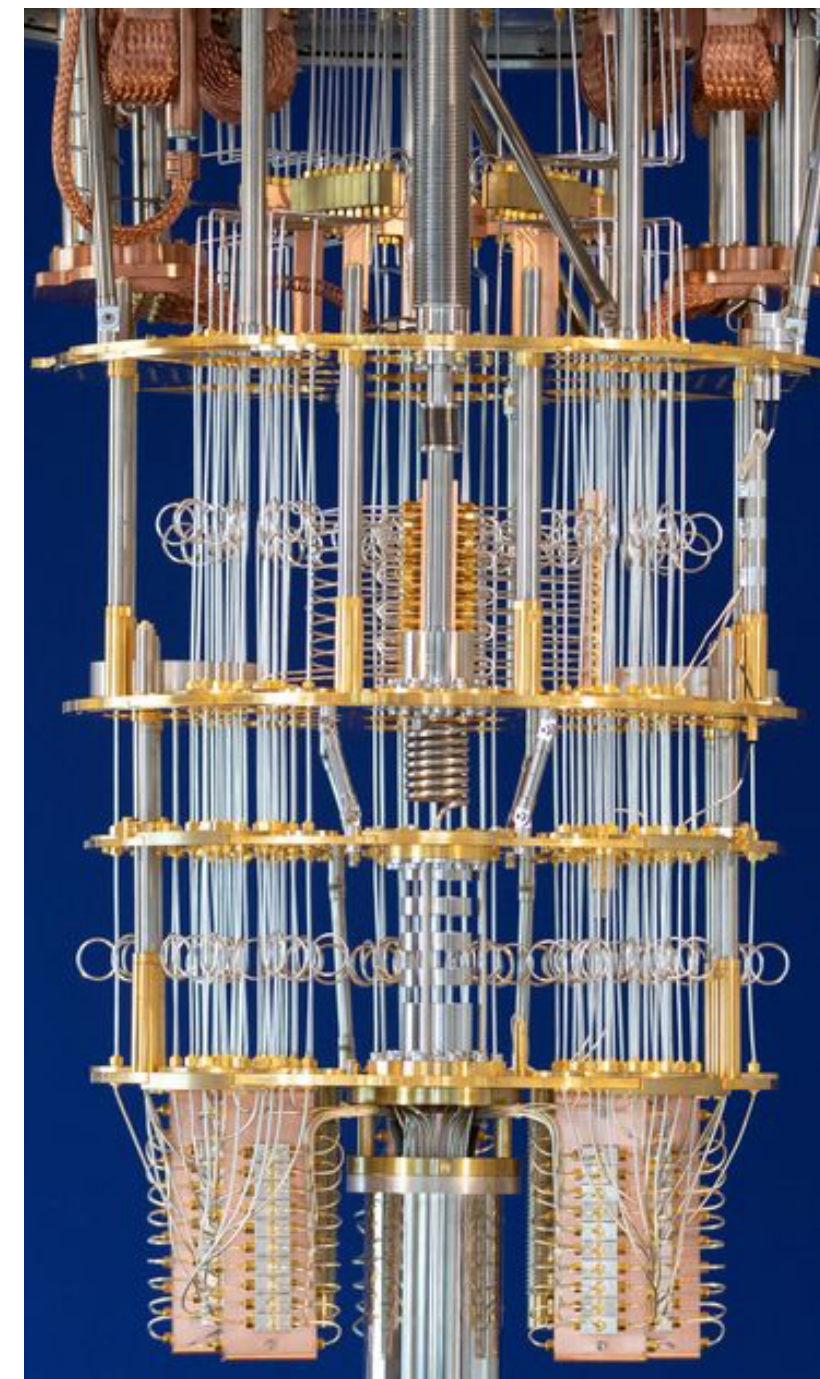
arXiv:1910.07596

Giuseppe Carleo (Flatiron Institute)

Antonio Mezzacapo (IBM)

Guglielmo Mazzola (IBM)

IBM Q



Chemistry simulations on a quantum computer

Second-quantized fermionic Hamiltonian with N orbitals:

$$\hat{H} = \sum_{\alpha, \beta=1}^N t_{\alpha\beta} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta} + \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta=1}^N u_{\alpha\beta\gamma\delta} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta}^{\dagger} \hat{c}_{\gamma} \hat{c}_{\delta}$$

Using Gaussian basis set, the Hamiltonian terms scales as $O(N^4)$

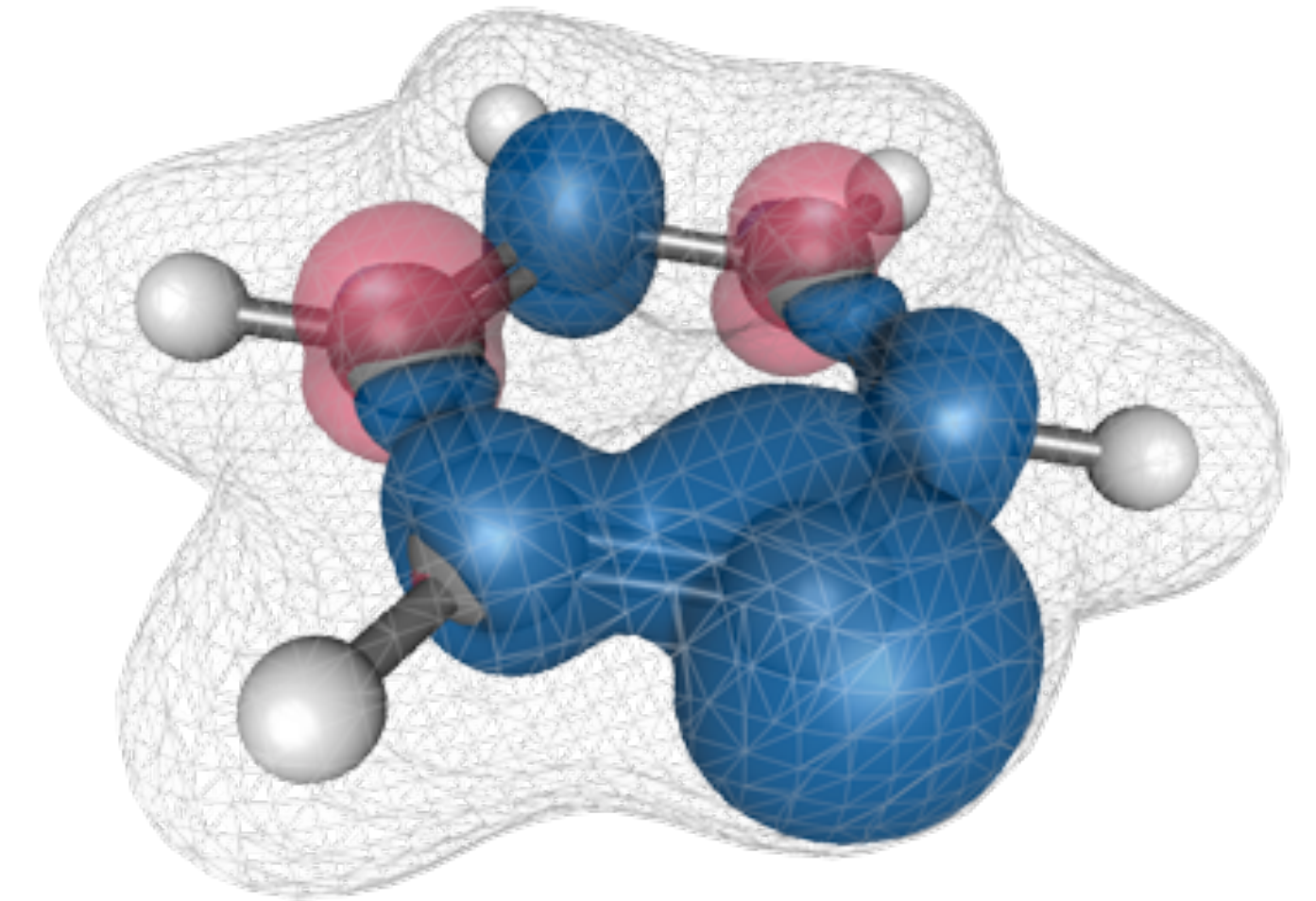
Map electronic orbitals to qubits (Jordan-Wigner, Bravyi-Kitaev, ...):

$$\hat{H} = \sum_{k=1}^K c_k \hat{P}_k \quad \hat{P}_k \in \{\mathbb{I}, \hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z\}^{\otimes N}$$

Ground state simulation: $\hat{H}|\Psi_0\rangle = E_0|\Psi_0\rangle$

Quantum phase estimation: precision can be systematically reduced, **deep circuits needed**.

Variational quantum simulation: hybrid quantum-classical, NISQ-friendly, **measurement-intensive**.



Variational quantum eigensolver

State preparation

$$|\Psi(\boldsymbol{\theta})\rangle = \hat{U}(\boldsymbol{\theta})|0\rangle^{\otimes N}$$

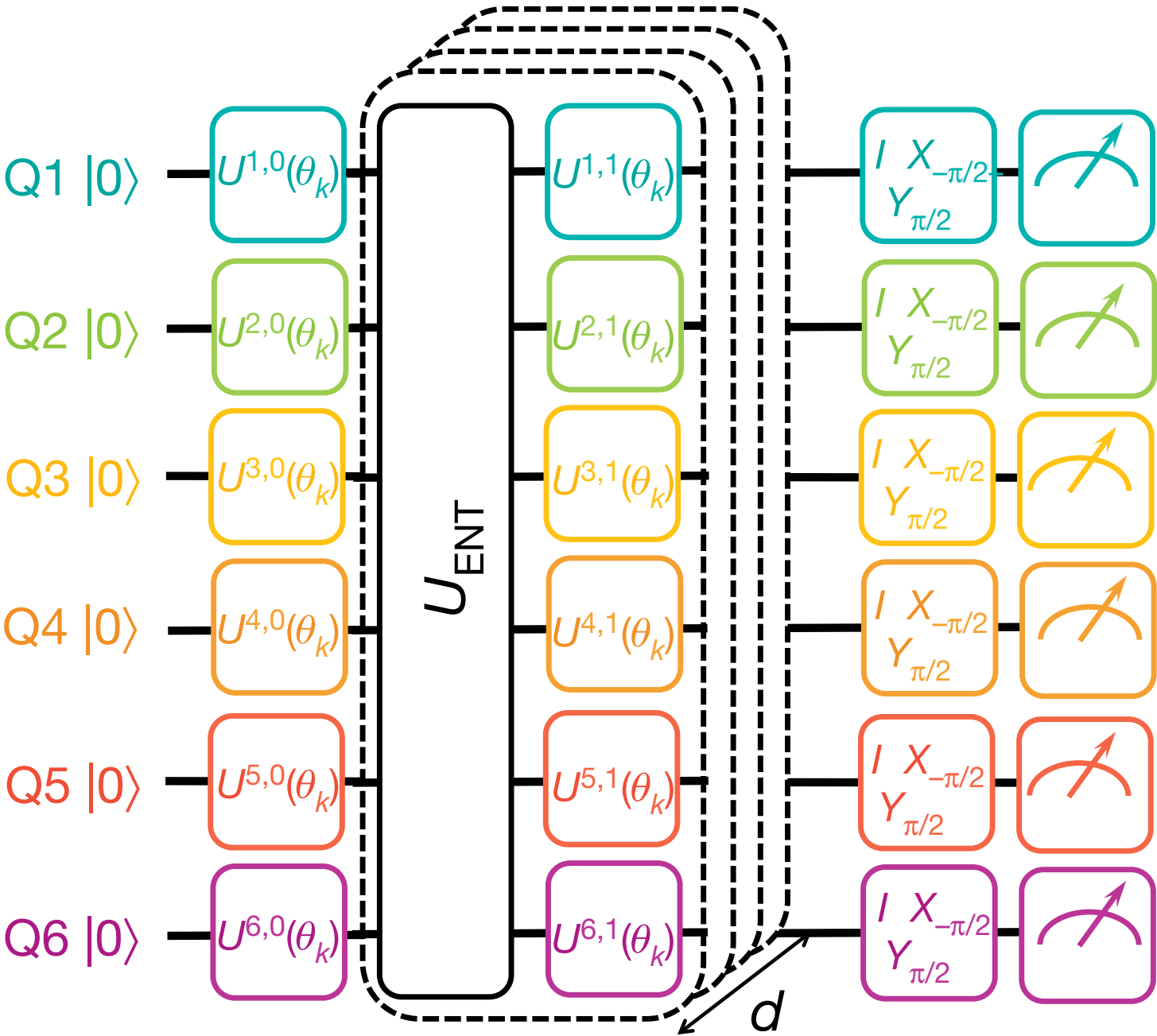
Evaluation of energy

$$E(\boldsymbol{\theta}) = \langle \Psi(\boldsymbol{\theta}) | \hat{H} | \Psi(\boldsymbol{\theta}) \rangle$$

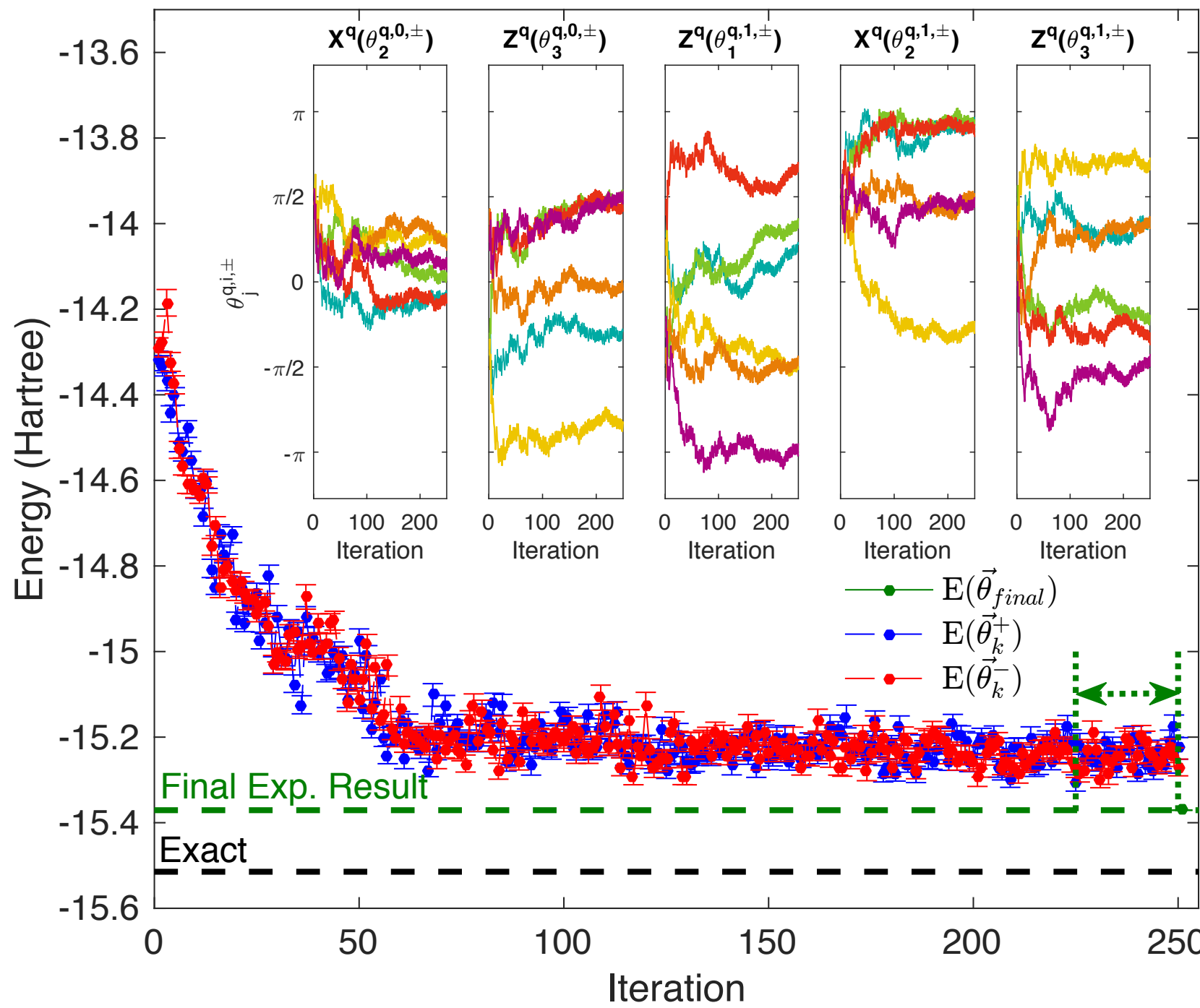
Circuit update

$$\Delta\boldsymbol{\theta} = -\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta})$$

Circuit Ansatz



Beryllium Hydrate



Intrinsic quantum noise

Consider energy measurement for exact ground state preparation: $|\Psi_0\rangle$

Energy measurement: $E_0 = \langle \Psi_0 | \hat{H} | \Psi_0 \rangle$ $\sigma^2[H] = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = 0$

Cannot measure in the energy eigenbasis!

$$\langle \hat{H} \rangle_{\text{qc}} = \sum_{k=1}^K c_k \langle \hat{P}_k \rangle \approx E_0 \quad \sigma^2[H]_{\text{qc}} = \sum_{k=1}^K |c_k|^2 \sigma^2[P_k]$$

$$\sigma^2[P_k] = \frac{1 - \langle \hat{P}_k \rangle^2}{S} \quad S = \# \text{ samples per Pauli}$$

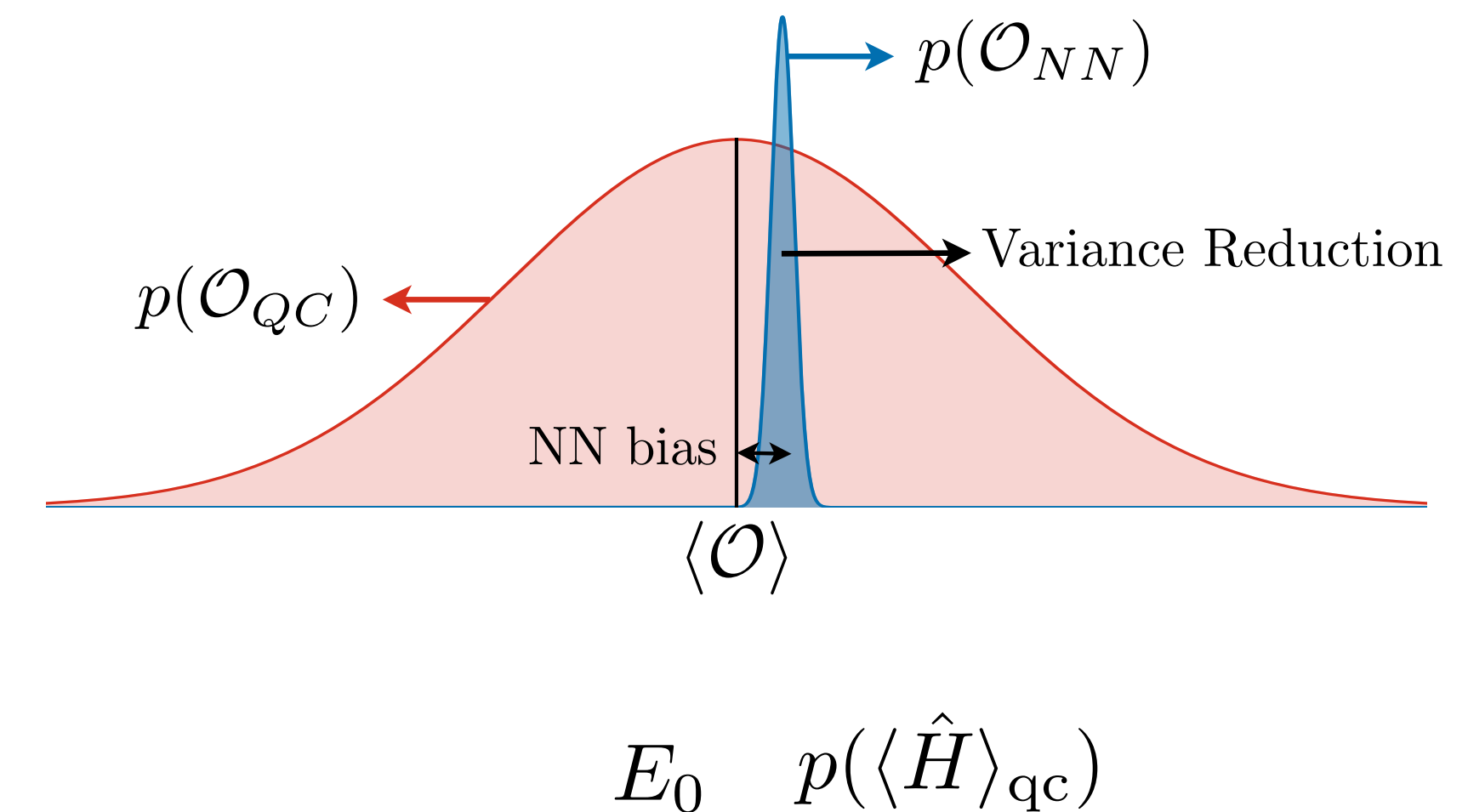
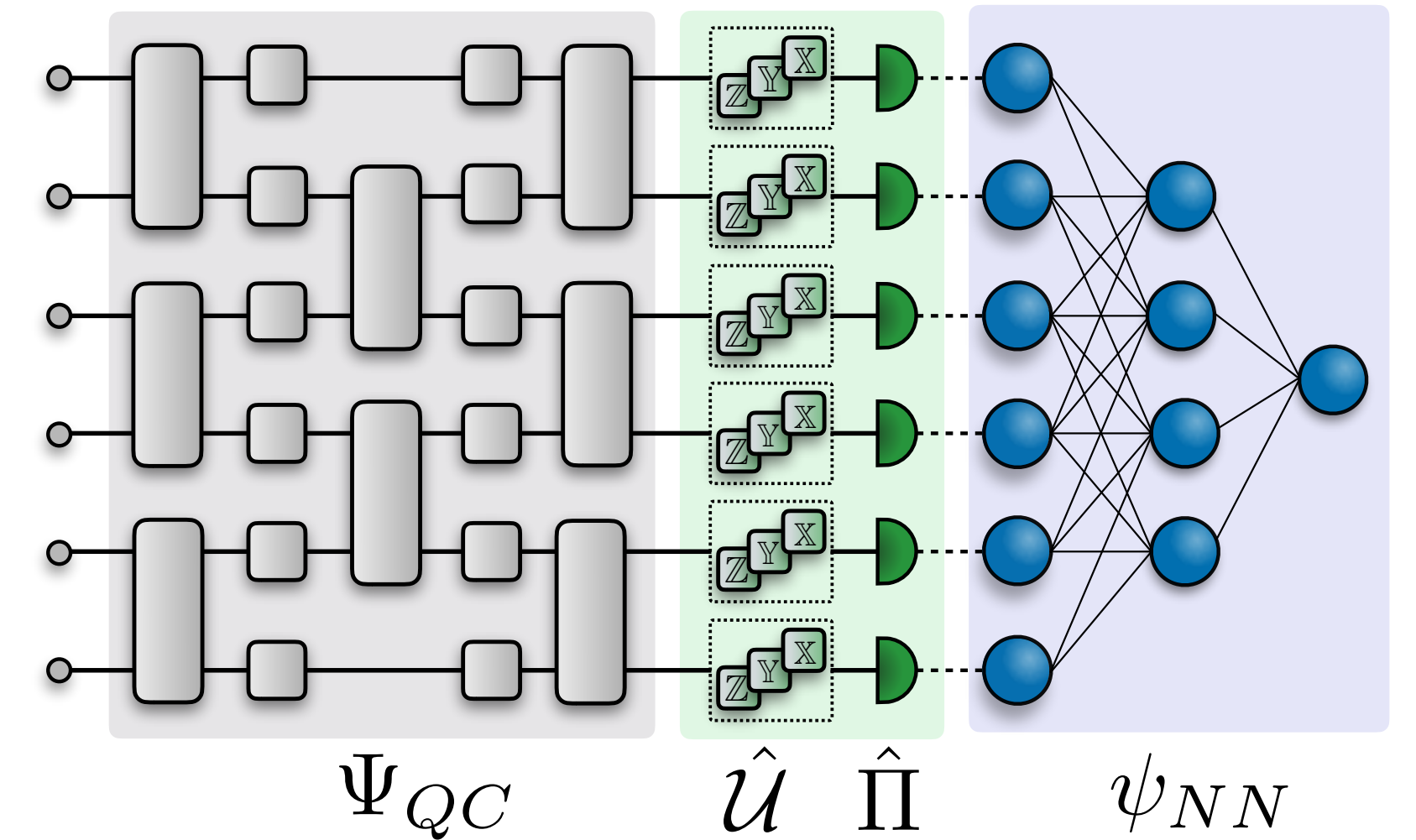
$$\text{Final uncertainty: } \epsilon_{\text{qc}} = \sqrt{\frac{\sum_k |c_k|^2 \sigma^2[P_k]}{S}}$$

Strategy: learn the quantum state from the same measurements instead.

$$\psi_{\lambda} \approx \Psi_0 \quad \longrightarrow \quad \langle \hat{H} \rangle_{\lambda} = \langle \psi_{\lambda} | \hat{H} | \psi_{\lambda} \rangle \approx \langle \hat{H} \rangle_{\text{qc}}$$

Neural-network measurement equivalent gathers statistics in the eigen-basis:

$$\sigma^2[H]_{\lambda} = \frac{\langle \hat{H}^2 \rangle_{\lambda} - \langle \hat{H} \rangle_{\lambda}^2}{n_{mc}} \approx 0$$



Quantum reconstruction of a fermionic wavefunction

Target wavefunction: $\Psi(\boldsymbol{\sigma}) \in \mathbb{C}$

Neural-network wavefunction: $\psi_{\boldsymbol{\lambda}}(\boldsymbol{\sigma}) \propto \sum_{\boldsymbol{h}} e^{-E_{\boldsymbol{\lambda}}(\boldsymbol{\sigma}, \boldsymbol{h})} \quad \boldsymbol{\lambda} \in \mathbb{C}$

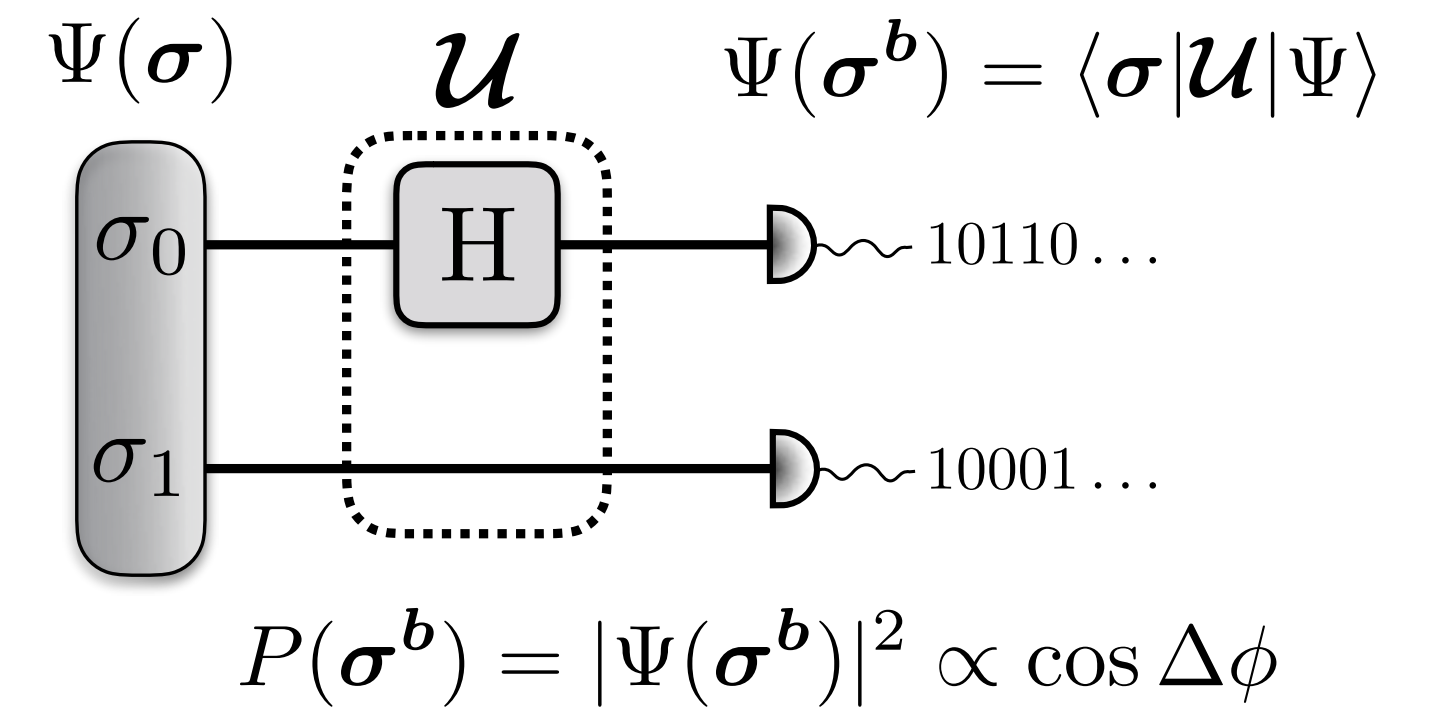
Reconstruction required data from many bases $|\boldsymbol{\sigma}^b\rangle = |\sigma_1^{b_1}, \sigma_2^{b_2}, \dots, \sigma_N^{b_N}\rangle$

Optimize an extended statistical divergence: $C_{\boldsymbol{\lambda}} = - \sum_{\boldsymbol{\sigma}^b \in \mathcal{D}} -\log |\psi_{\boldsymbol{\lambda}}(\boldsymbol{\sigma}^b)|^2$

Using single-qubit Pauli rotations $\hat{\mathcal{U}}$:

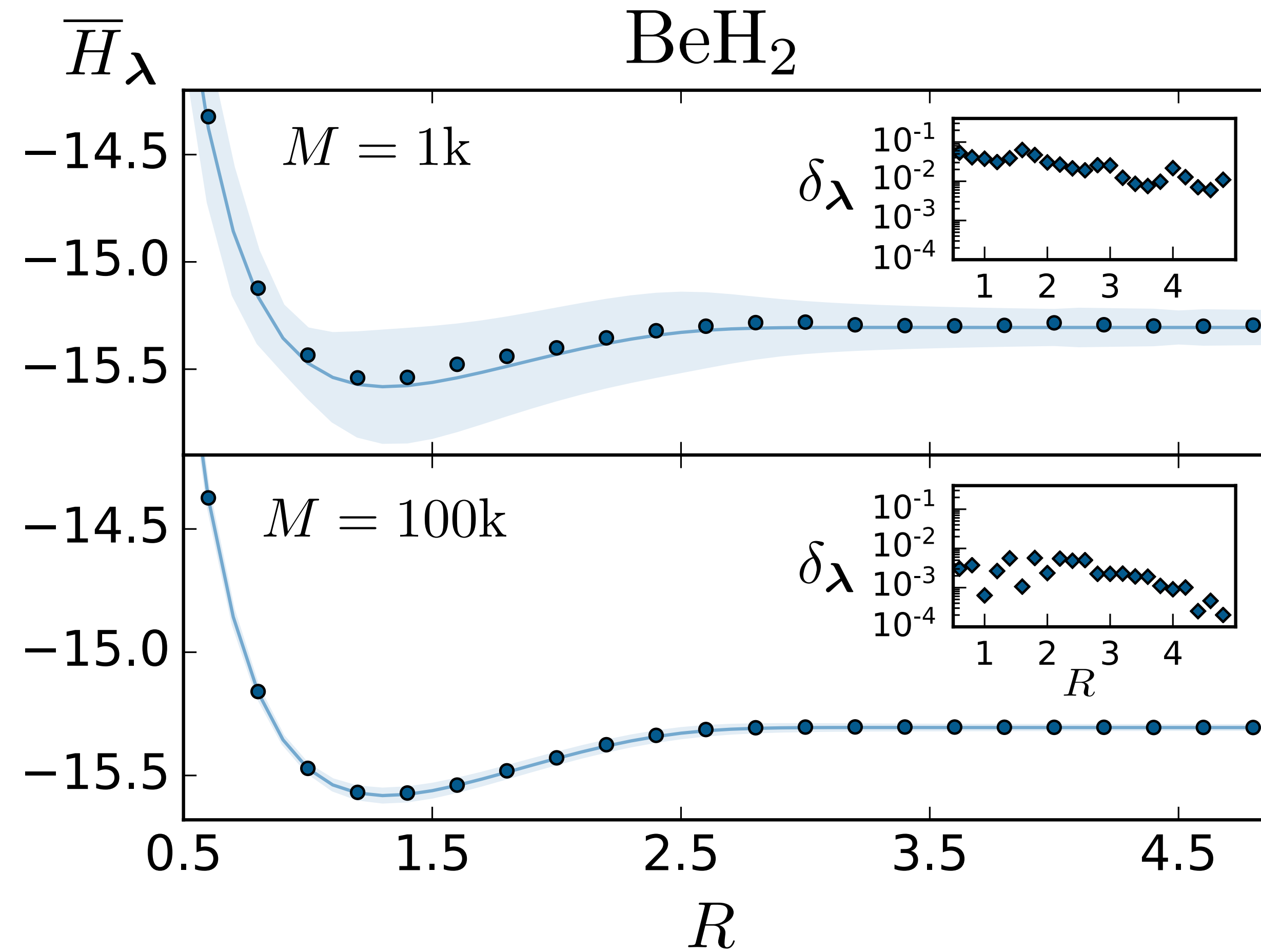
$$\begin{aligned} \psi_{\boldsymbol{\lambda}}(\boldsymbol{\sigma}^b) &= \sum_{\boldsymbol{\sigma}} \mathcal{U}_{\boldsymbol{\sigma}, \boldsymbol{\sigma}^b} \psi_{\boldsymbol{\lambda}}(\boldsymbol{\sigma}) \quad \text{Restrict rotation to a set } \Lambda \text{ of } N_U \text{ qubits:} \\ &= \sum_{\boldsymbol{s}} \prod_{j \in \Lambda} \langle \sigma_j^{b_j} | \sigma_j \rangle \left[\bigotimes_{\ell \notin \Lambda} \langle \sigma_{\ell} | \otimes \langle \boldsymbol{s} | \right] |\psi_{\boldsymbol{\lambda}}\rangle \quad O(2^{N_U}) \end{aligned}$$

For reconstructing energy measurements on the ground state, only Pauli bases in the Hamiltonian are required.



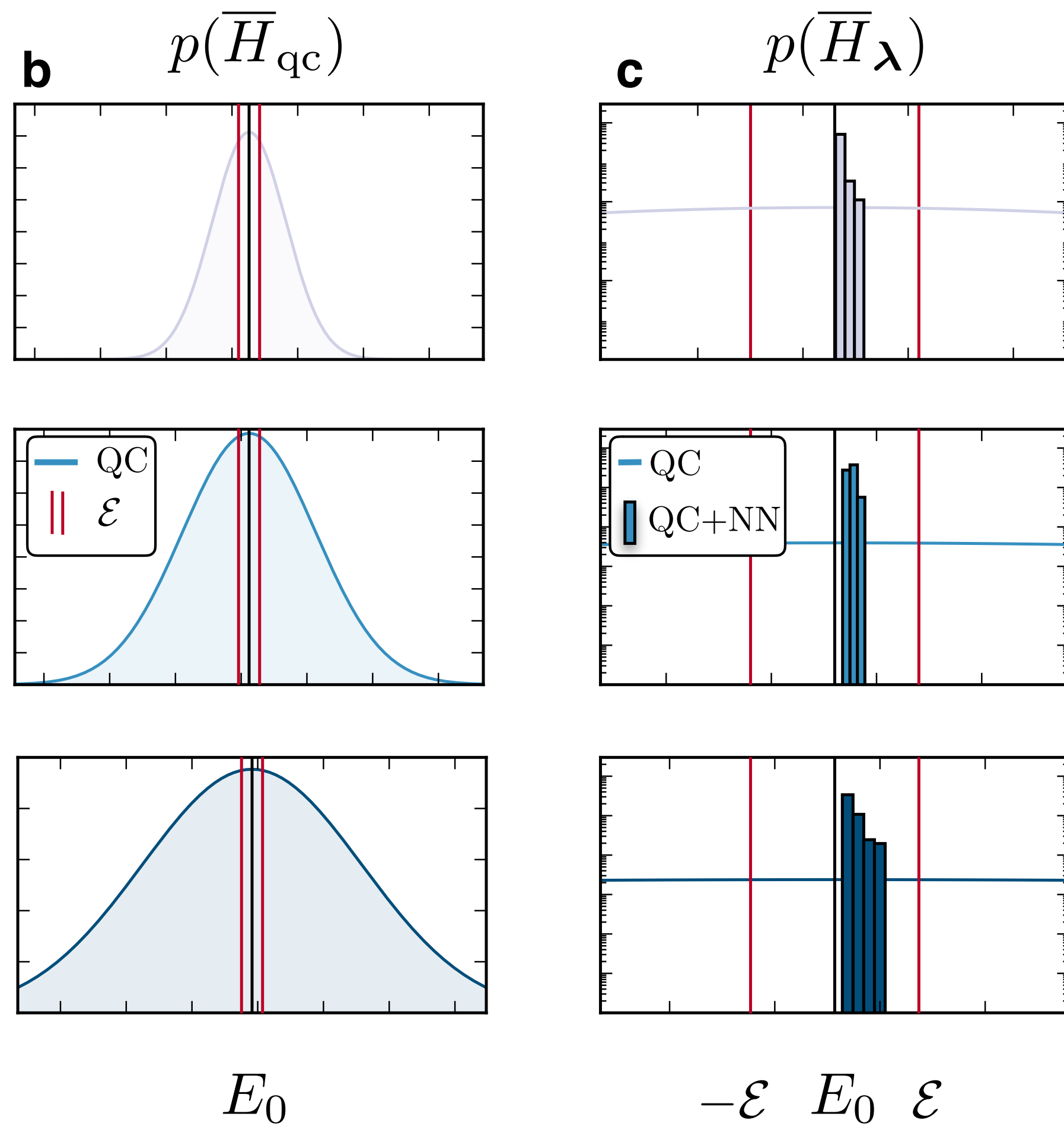
Energy measurements

Dissociation energy profile

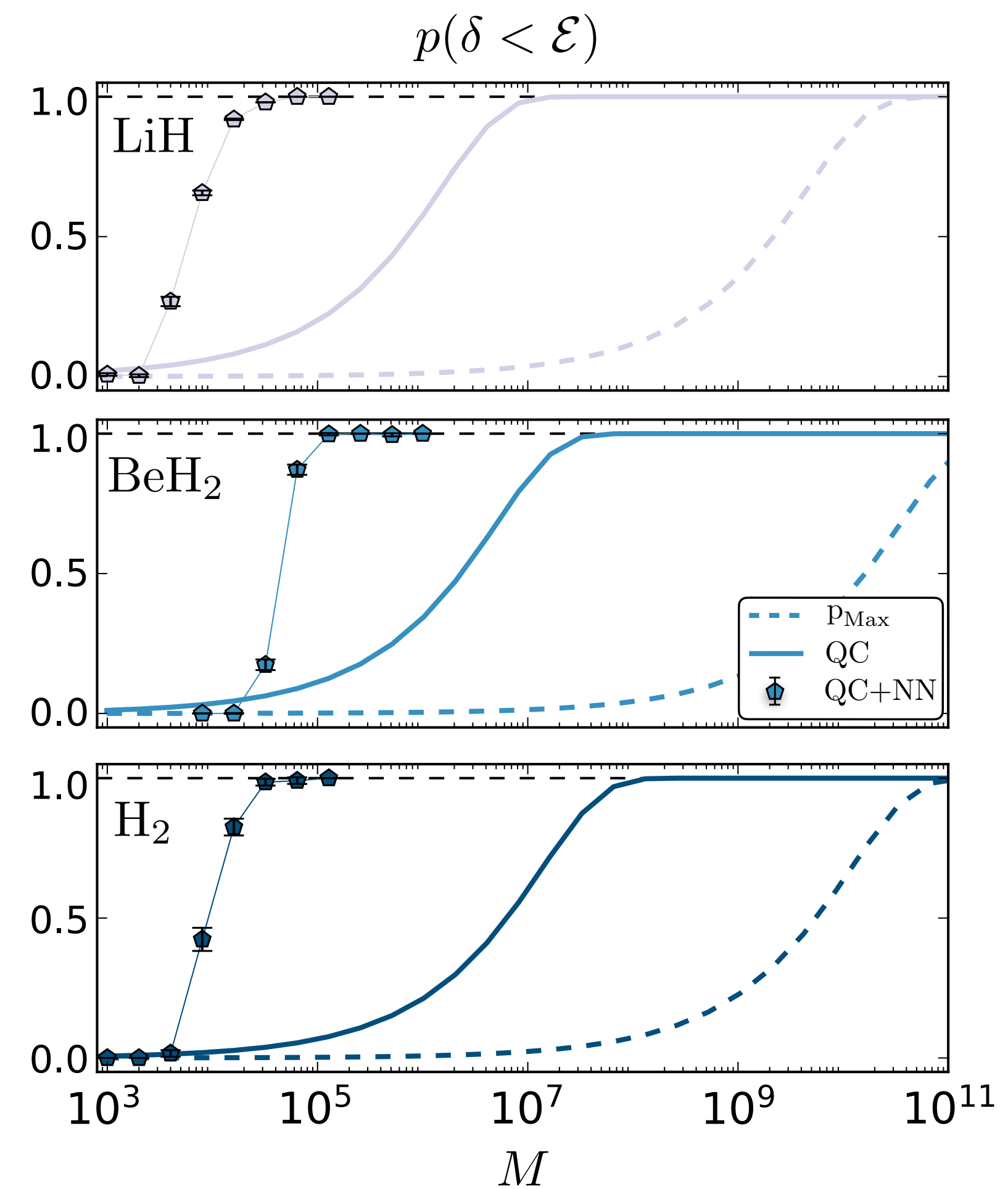


Energy measurements

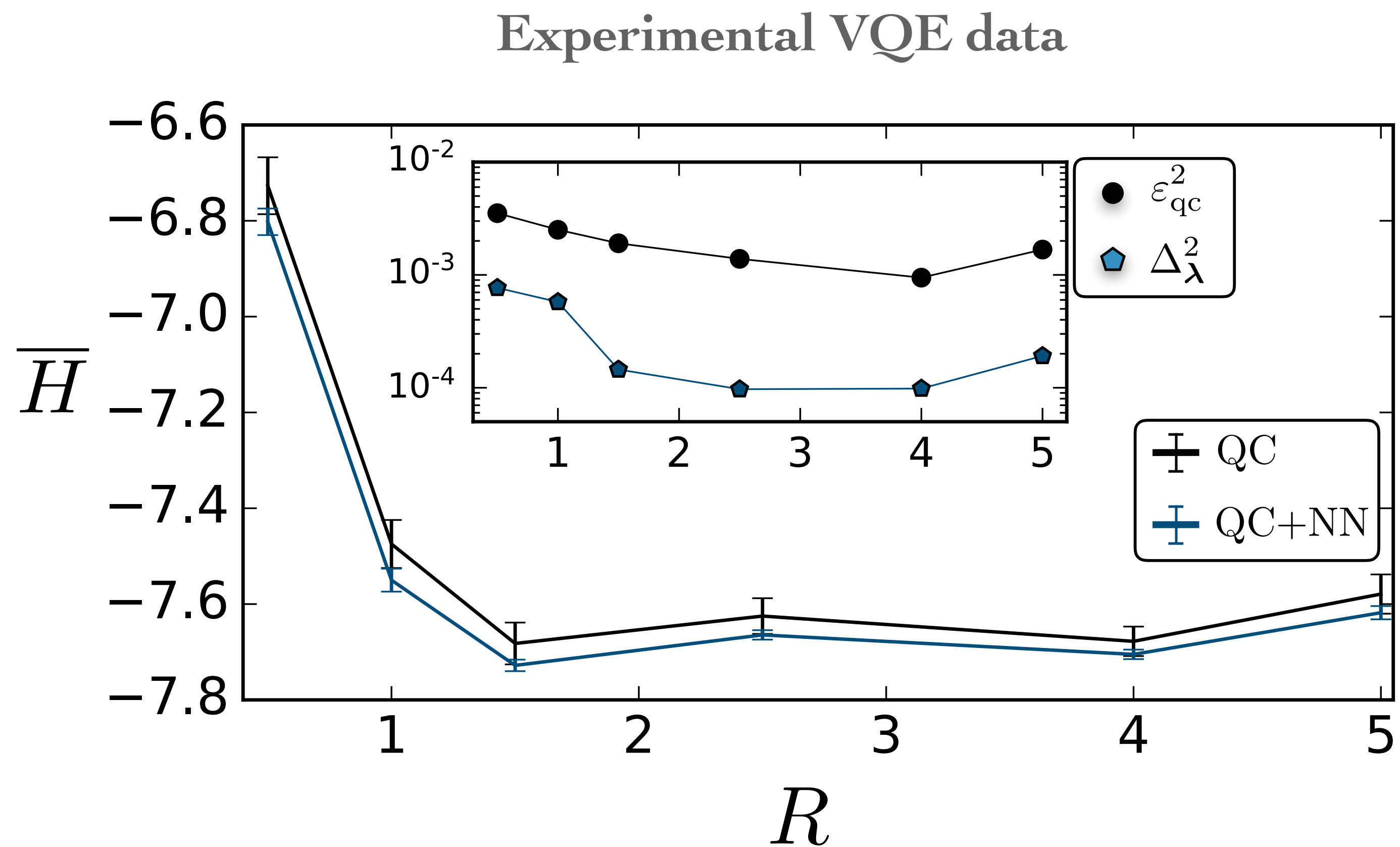
Energy estimator distribution



Chemical accuracy probability



Neural-network estimators

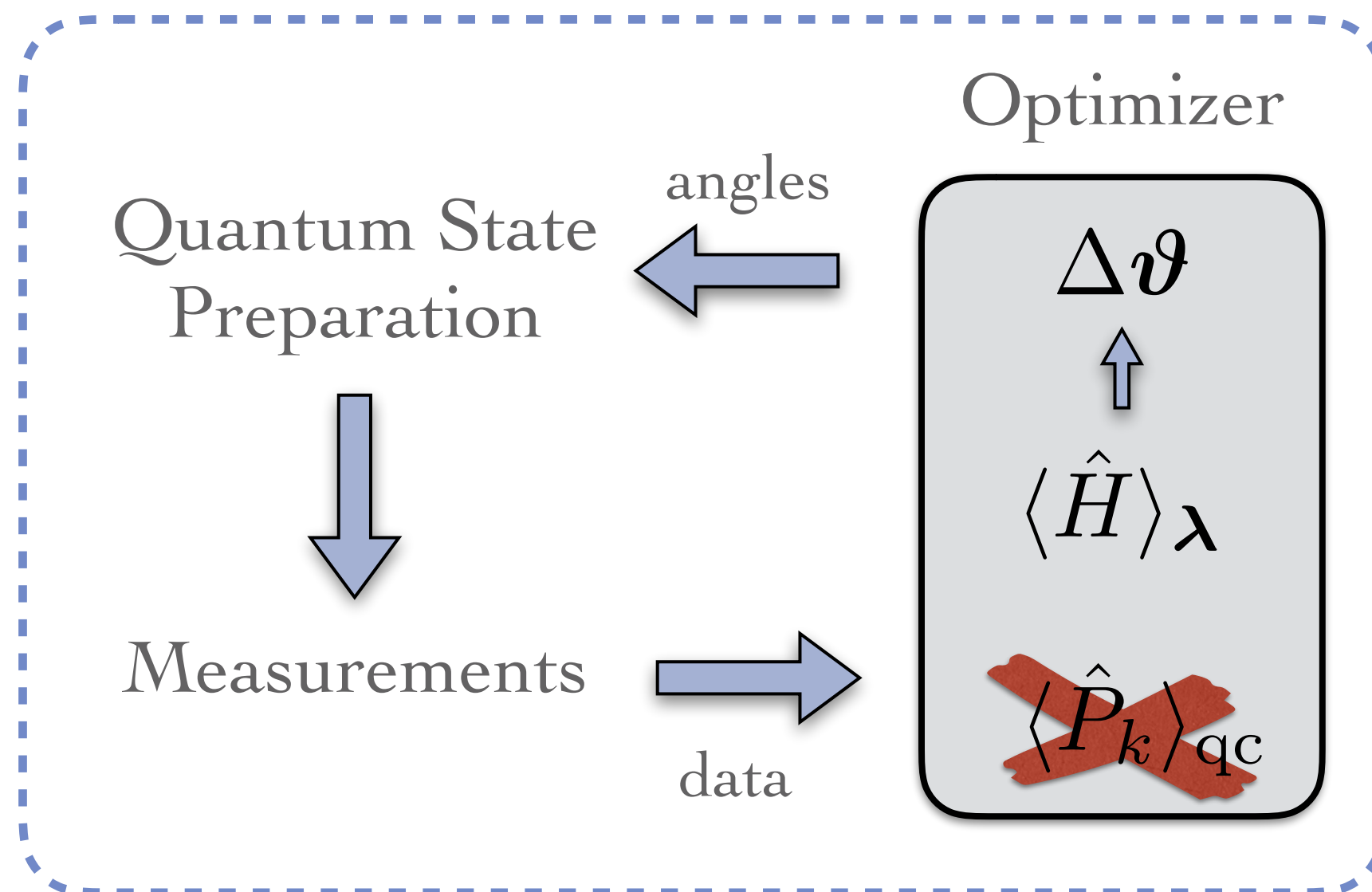


Reconstruction with 5000 measurements
(out of the 2.5 millions)

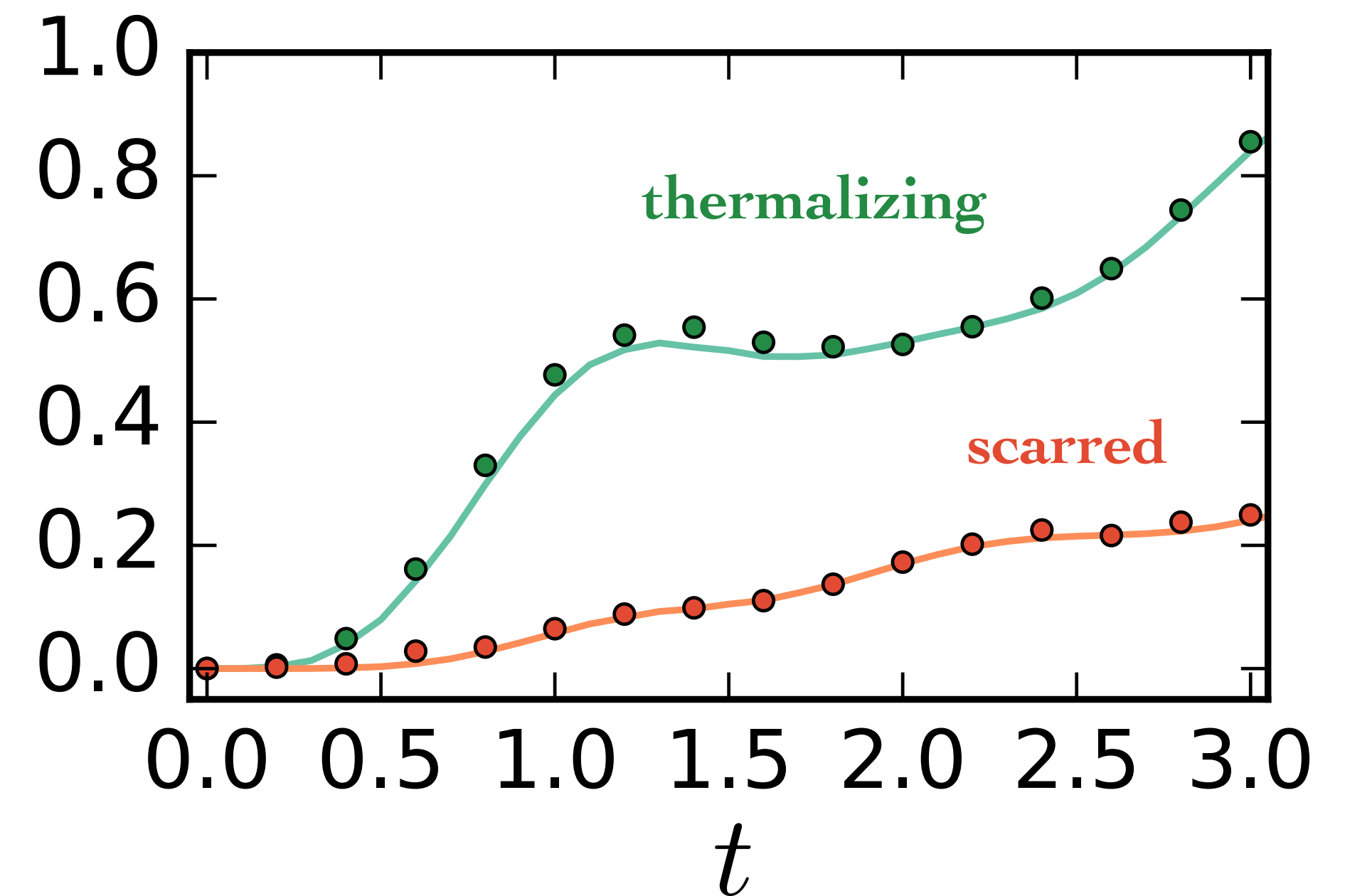
Outlook

Generative Modeling of Experimental Wavefunctions

VQE Embedding



Quantum Dynamics



Entanglement entropy after a quench

- Learnability theory of quantum states
Sehayek *et al*, Physical Review B (2019)
- Reconstruction of quantum-supreme wavefunctions (verification?)