Quantum simulation with Rydberg atom arrays

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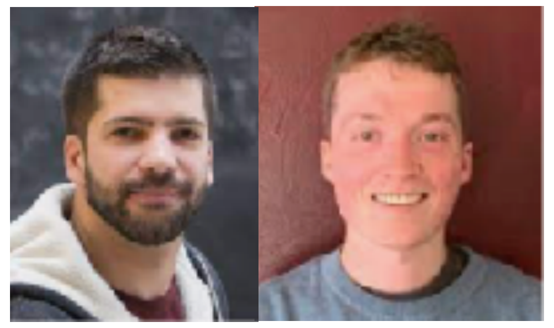
PERIMETER INSTITUTE

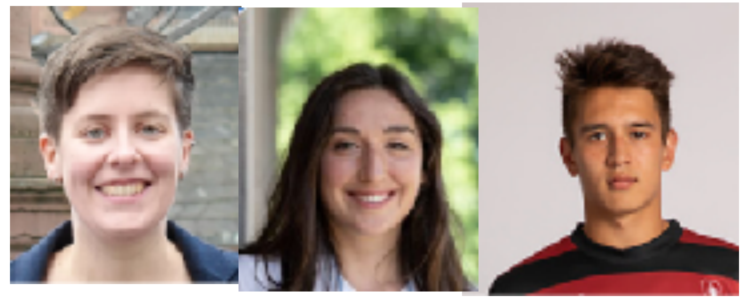
Integrating Neural Networks with a Quantum Simulator for State Reconstruction
G. Torlai, B. Timar, E. van Nieuwenburg, H. Levine, A. Omran, A. Keesling, H. Bernien, M. Greiner, V. Vuletić, M. Lukin, RGM, and M. Endres, Phys. Rev. Lett. 123, 230504 (2019)



Stochastic Series Expansion Quantum Monte Carlo for Rydberg Arrays
E. Merali, I. De Vlugt, RGM, arXiv: 2107.00766 (Scipost)

Bulk and Boundary Quantum Phase Transitions in a Square Rydberg Atom Array
M. Kalinowski, R. Samajdar, RGM, M. Lukin, S. Sachdev, S. Choi, arXiv:2112.10790

Enhancing variational Monte Carlo with quantum data
S. Czischek, M. S. Moss, M. Radzihovsky, E. Merali and RGM



Outline

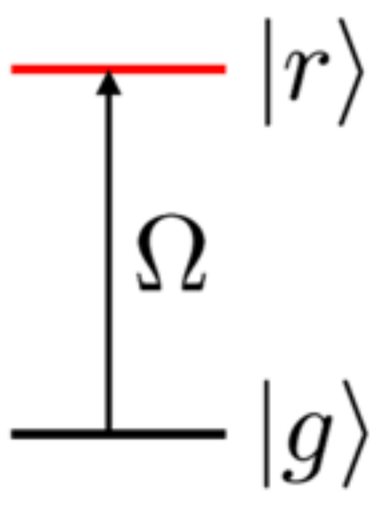
- Rydberg array quantum simulators/emulators
- *In silico* simulation strategies: DMRG, QMC
- Data-driven strategies: neural network wavefunctions & VMC

Rydberg atom arrays

- Neutral atoms (Rb, Sr) are loaded into a lattice formed by an array of optical tweezers
- Atoms can be in their ground state, or an excited state with a large principle quantum number (a Rydberg state). They form a strongly-interacting system.
- Single-atom resolved fluorescent imaging provides projective measurements
- Arrays of atoms are currently used for simulation (groundstates, critical phenomena), solving combinatorial optimization problems

Rydberg Blockade Hamiltonian

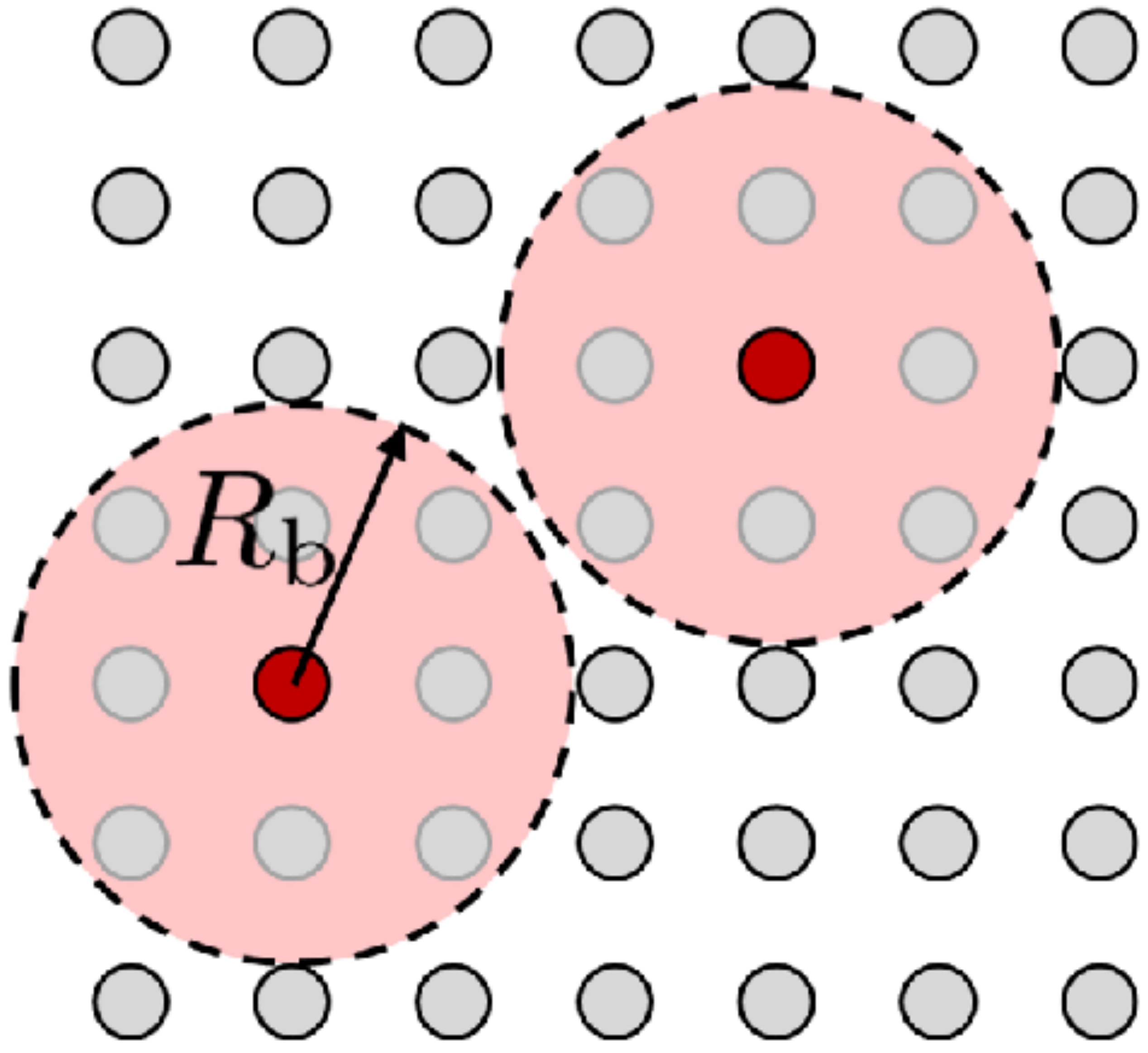
Jaksch, Cirac, Zoller, Rolston, Cote, Lukin, Phys. Rev. Lett. 85, 2208 (2000)
Lukin, Fleischhauer, Cote, Duan, Jaksch, Cirac, Zoller, Phys. Rev. Lett. 87, 037901 (2001)
Fendley, Sengupta, Sachdev, Phys. Rev. B 69, 075106 (2004)



$$H = \Omega \sum_i \sigma_i^x - \Delta \sum_i n_i + \sum_{i<j} V_{ij} n_i n_j$$

$$V(R) = \frac{\Omega}{(R/R_b)^6}$$

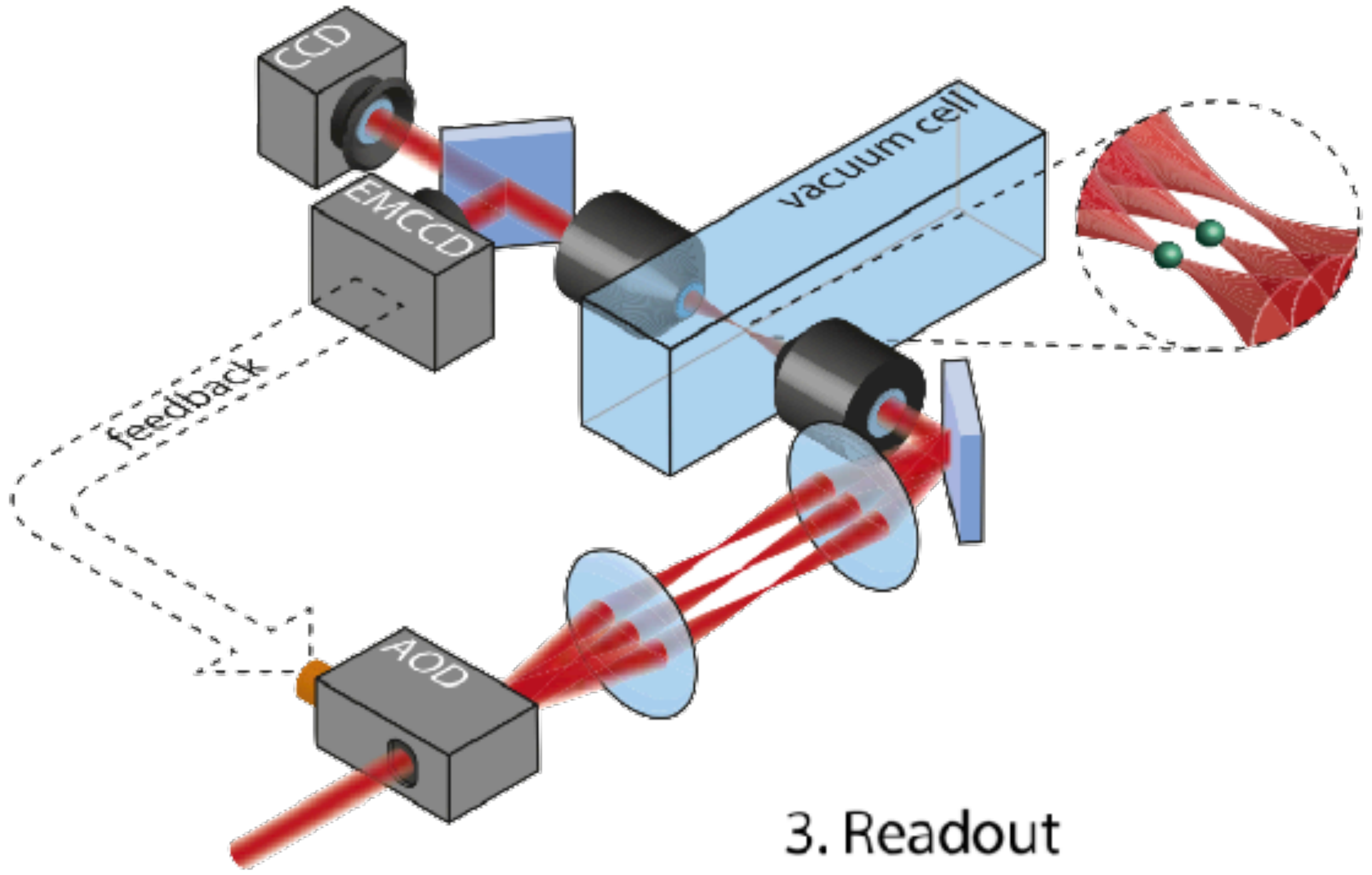
$$\sigma^x = |g\rangle\langle r| + |r\rangle\langle g| \qquad n = |r\rangle\langle r|$$



Browaeys, Lahaye, Nature Physics 16, 132 (2020)

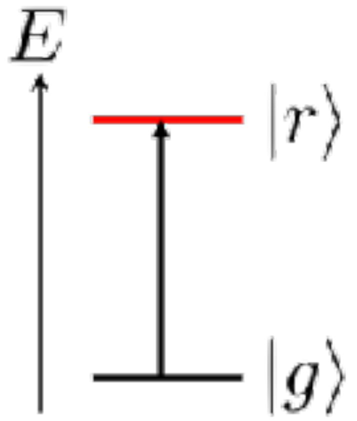
- Two atoms within the blockade radius cannot both be excited into a Rydberg state simultaneously
- Lattice geometry crucially affects physics

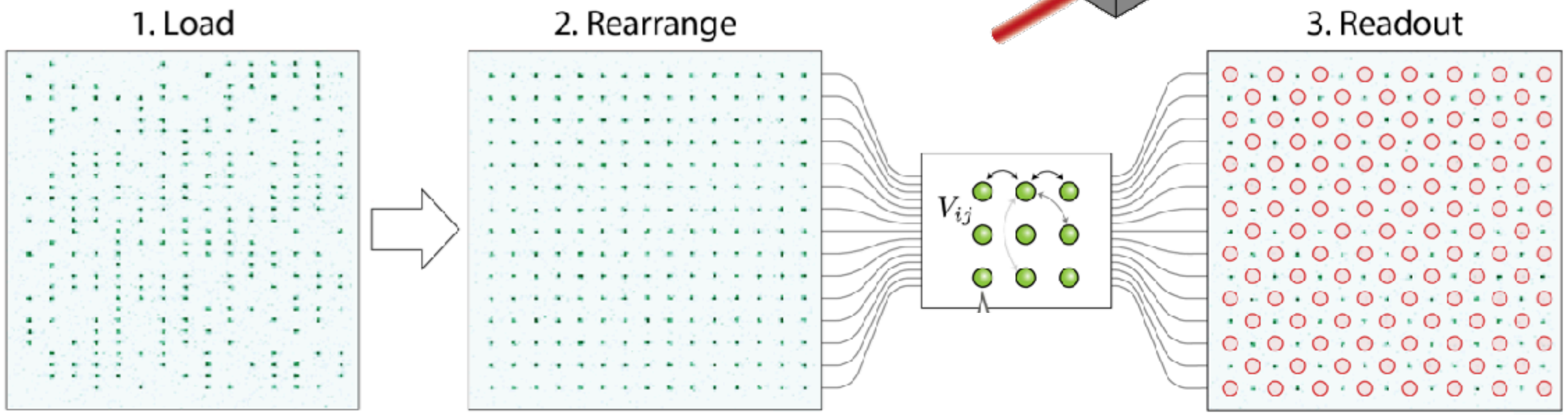
Experimental Rydberg Arrays

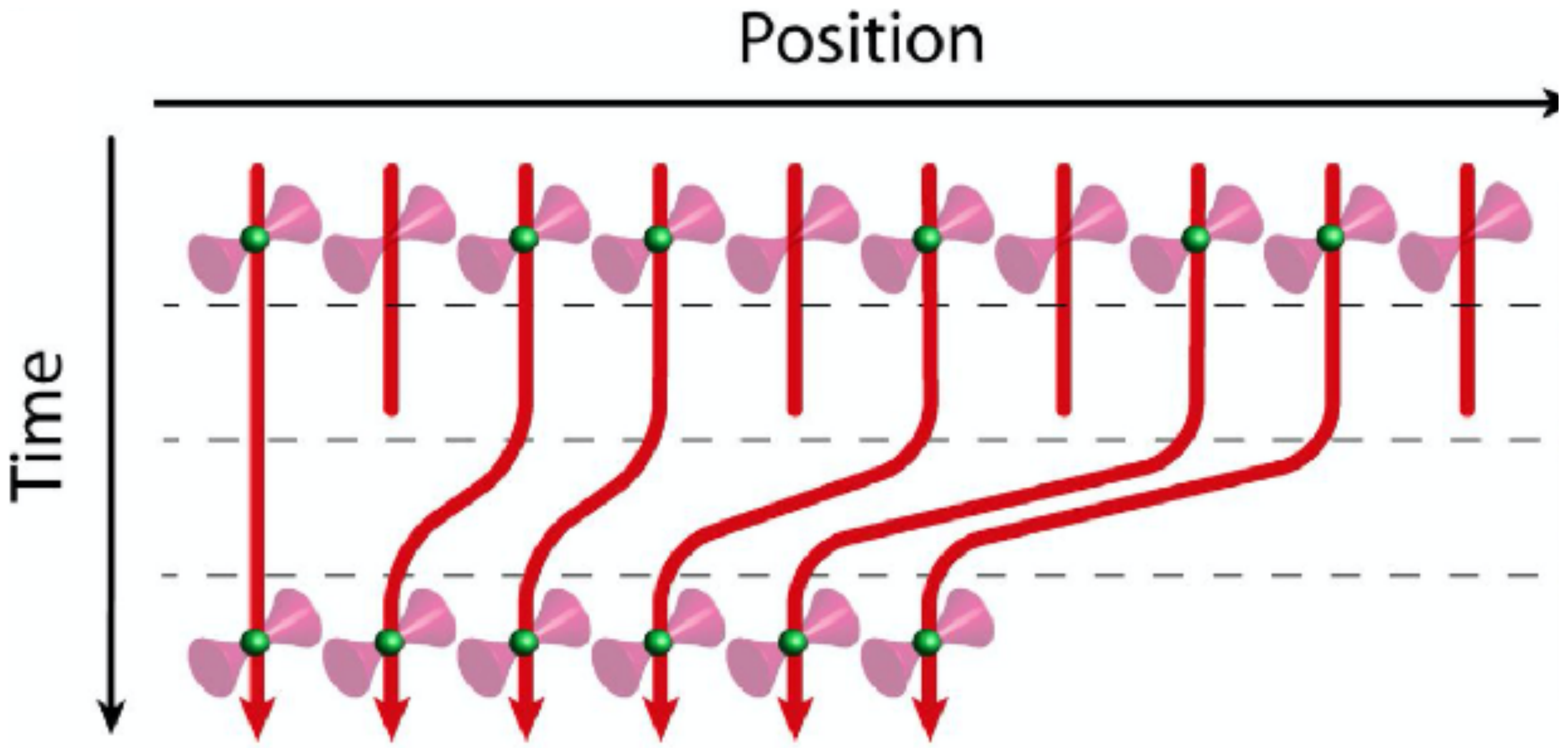


Ebadi et. al. arXiv:2012.12281
Nature 595, 227 (2021)

$^{87}\mathrm{Rb}$



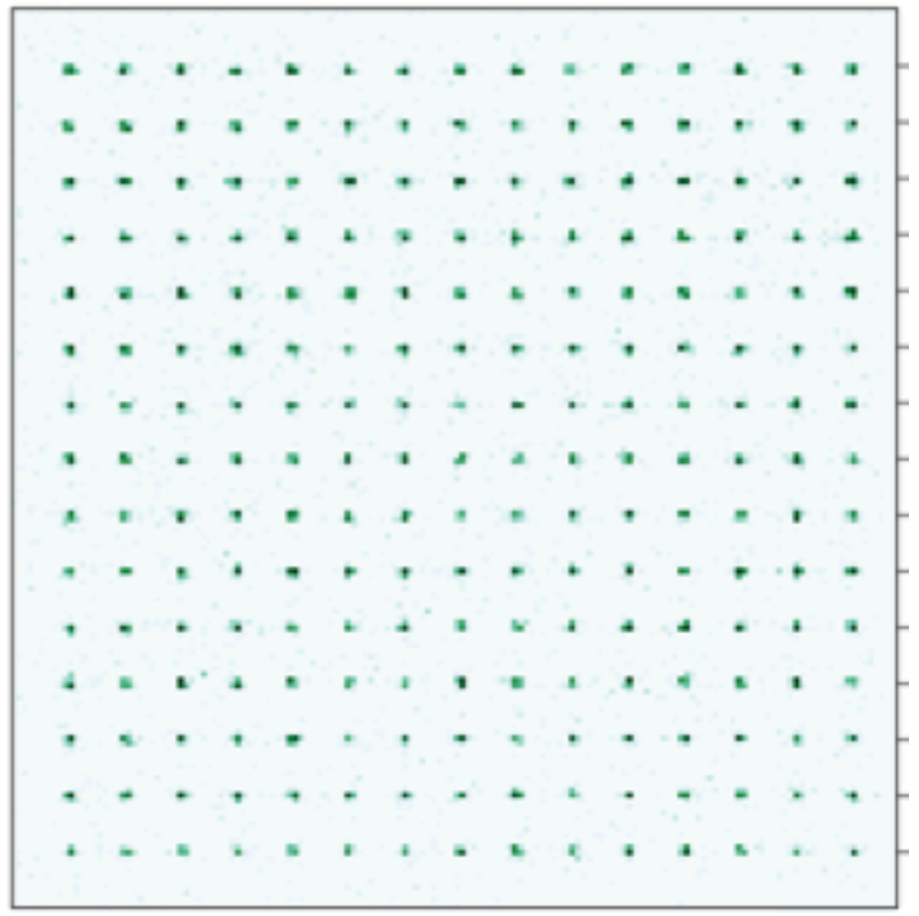




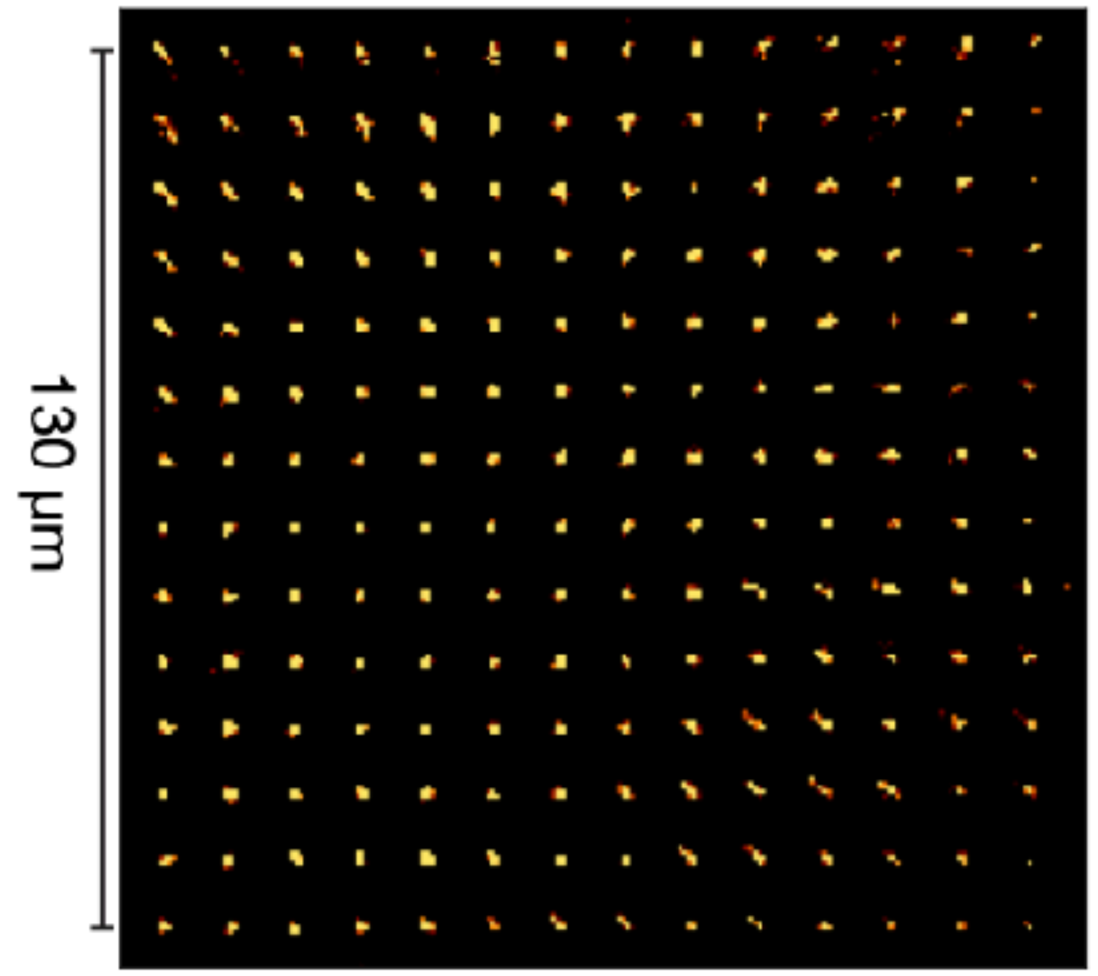
Single-atom resolved fluorescent imaging provides projective measurements of $|g\rangle$

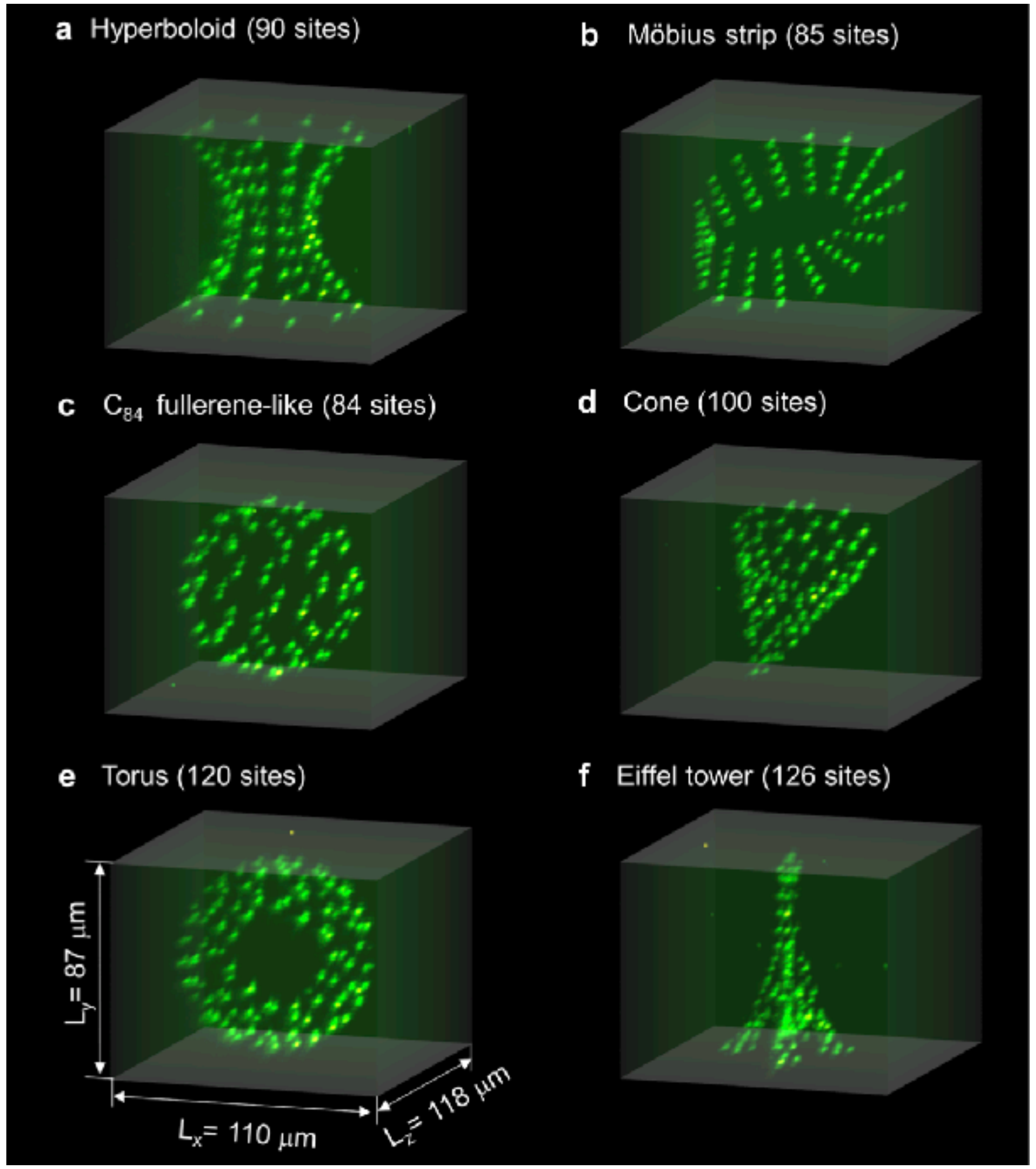
Endres et. al. Science 354, 1024 (2016)

Experimental lattices

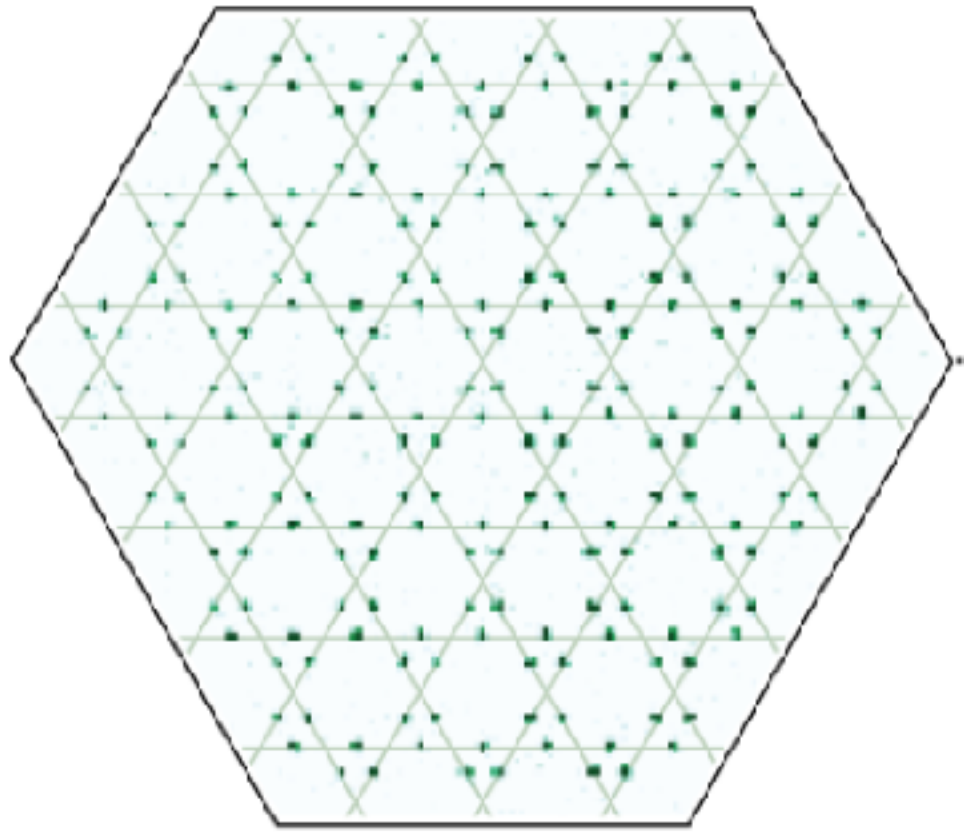


Ebadi et. al. arXiv:2012.12281
Nature 595, 227 (2021)

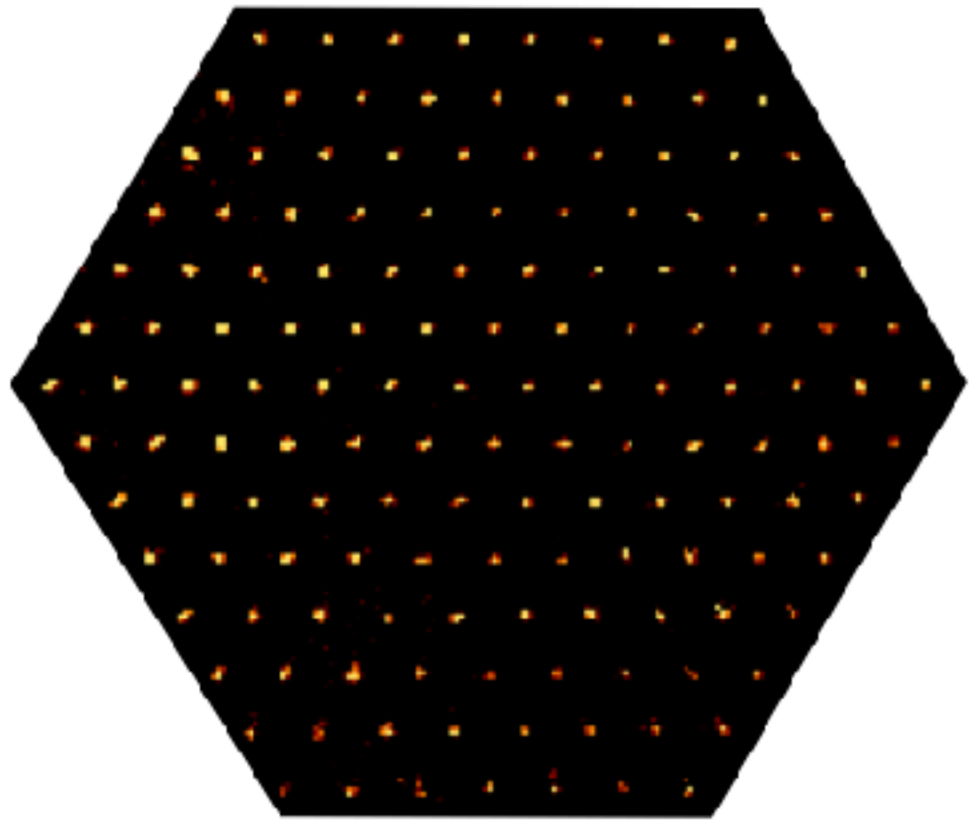




Barredo, Lienhard, de Léséleuc, Lahaye, Browaeys
Nature 561, (2018)



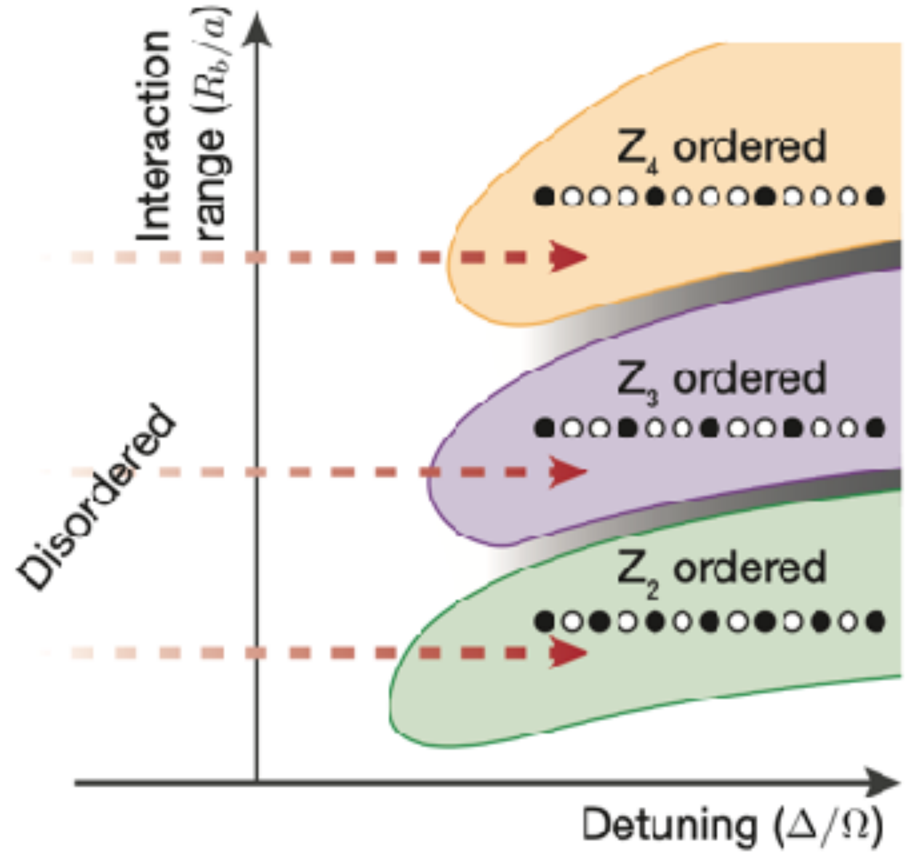
Semeghini et. al. arXiv:2104.04119
Science, 374, 1242 (2021)

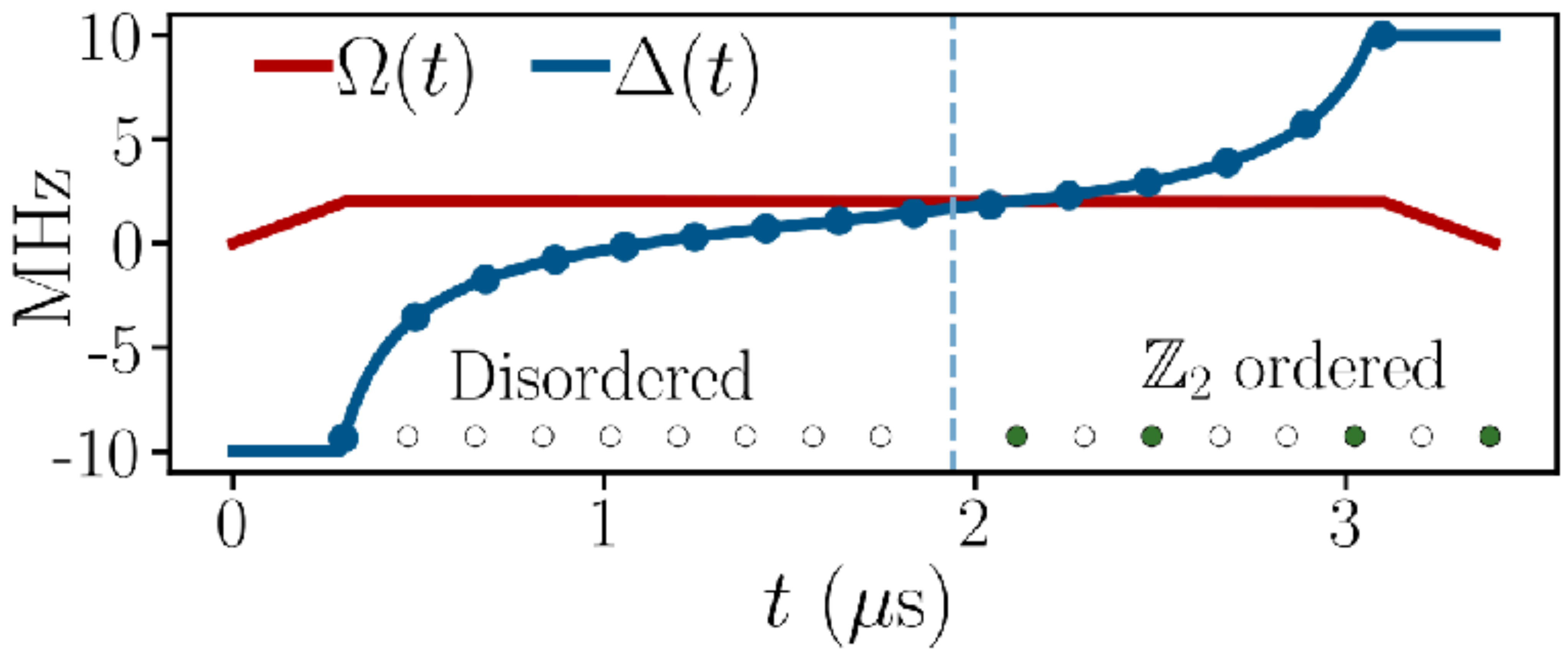


Scholl et al. arXiv:2012.12268
Nature 595, 233 (2021)

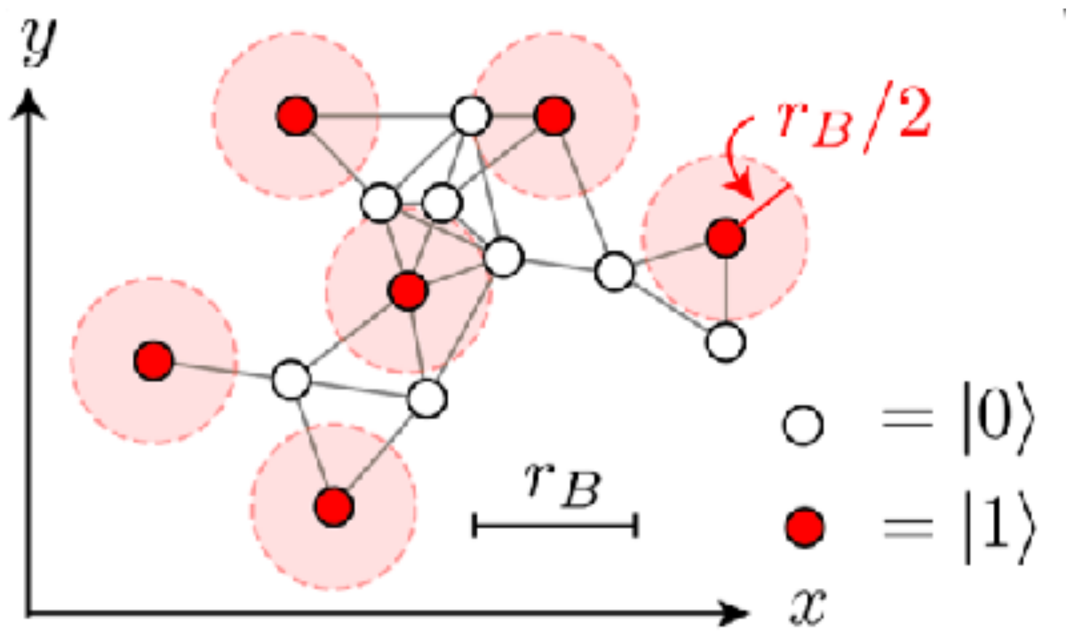
Adiabatic state preparation

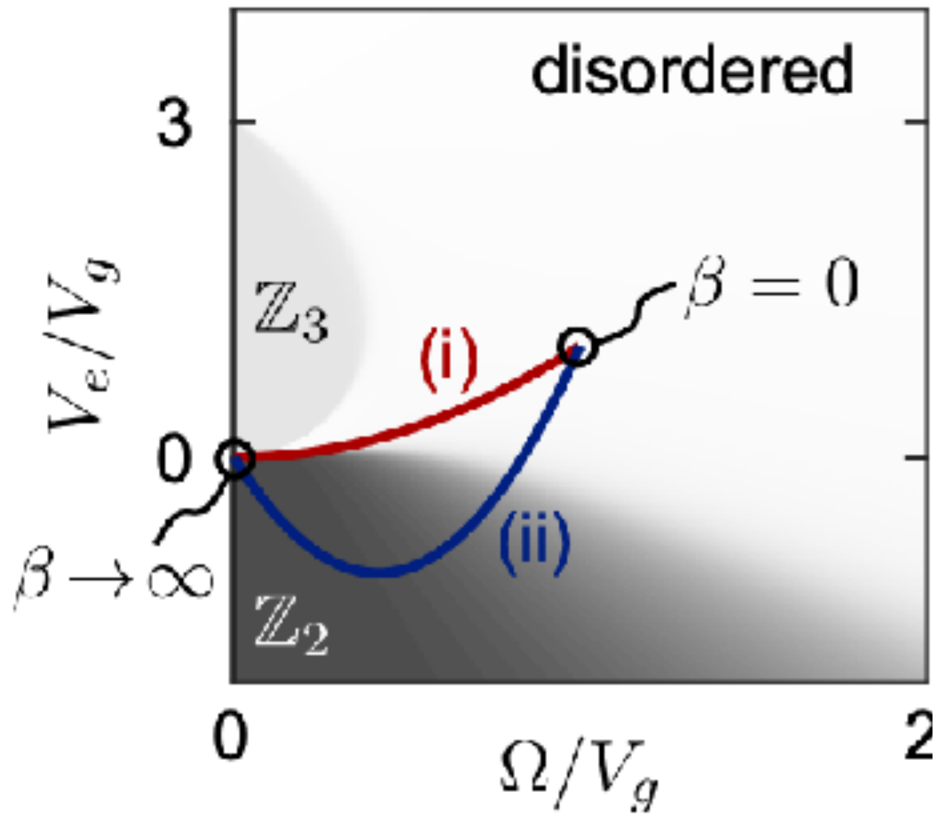
- Phase diagrams are studied by detuning across the bare resonance





- Optimization problems (MIS) and quantum sampling



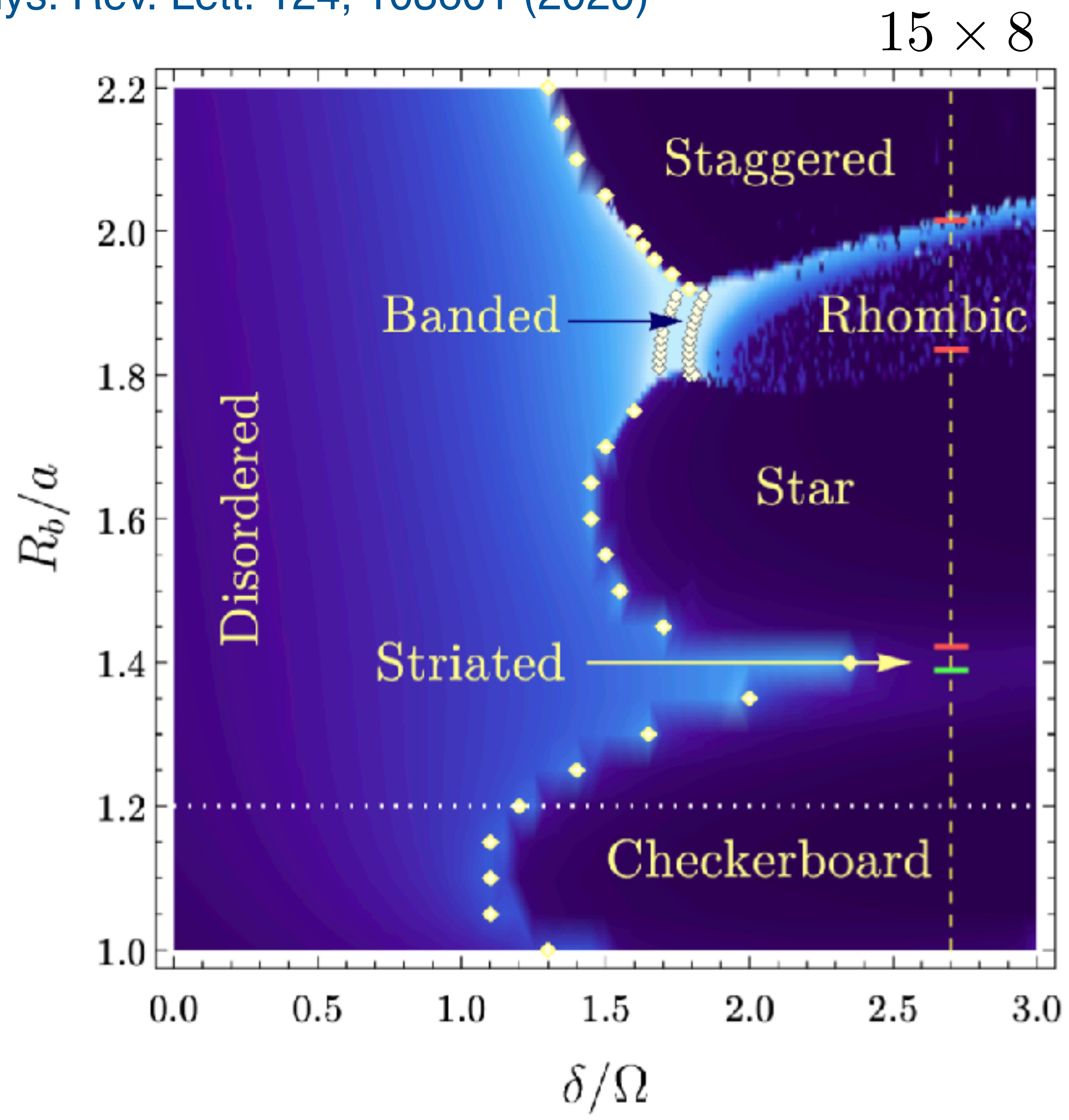


H. Pichler, S.-T. Wang, L. Zhou, S. Choi, and M. D. Lukin,
Quantum optimization for maximum independent set using Rydberg atom arrays, arXiv:1808.10816,
Computational complexity of the Rydberg blockade in two dimensions, arXiv:1809.04954

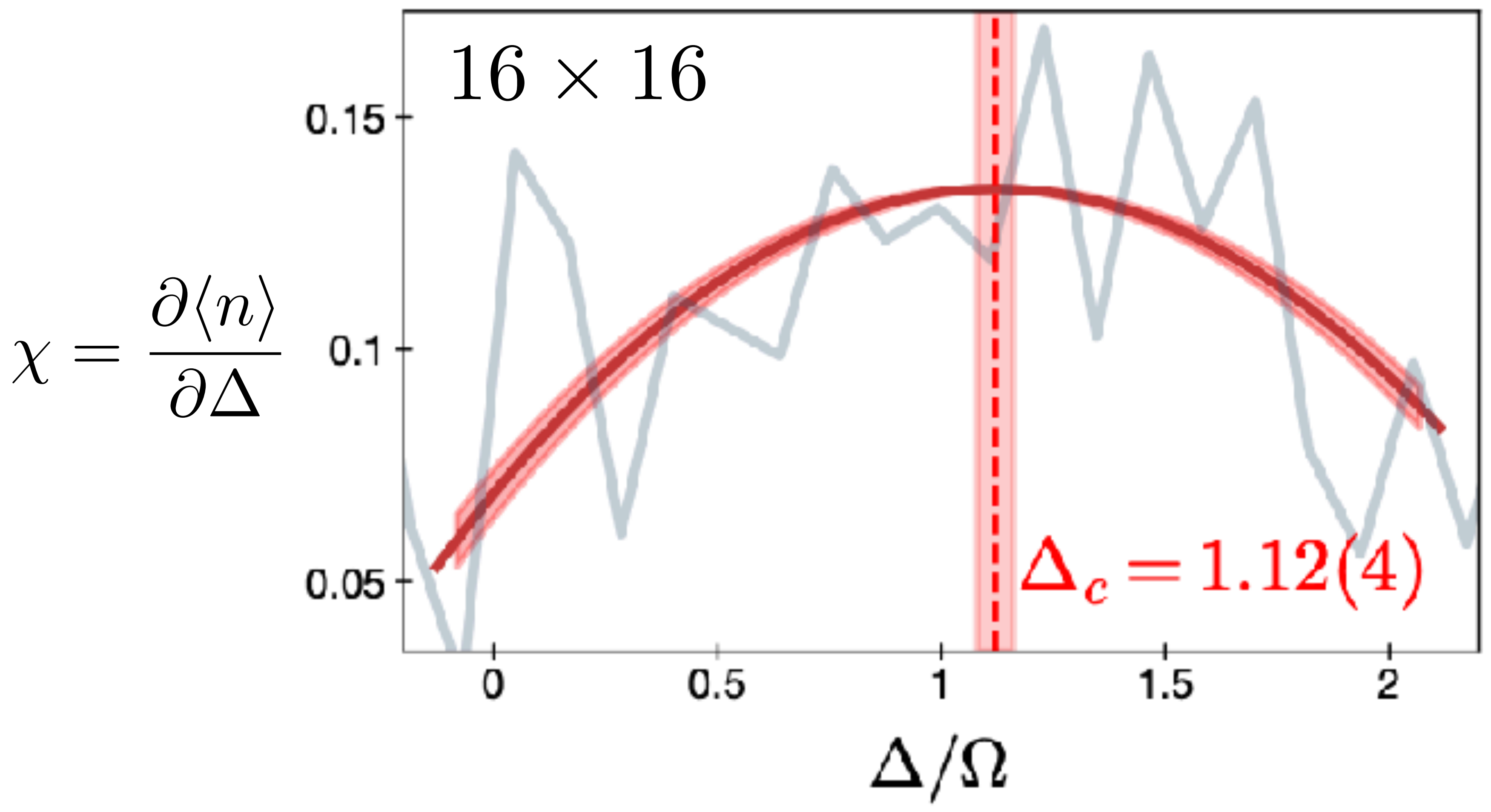
D. Wild, D. Sels, H. Pichler, C. Zanoci, M. Lukin
Quantum Sampling Algorithms for Near-Term Devices
arXiv:2005.14059, arXiv:2109.03007

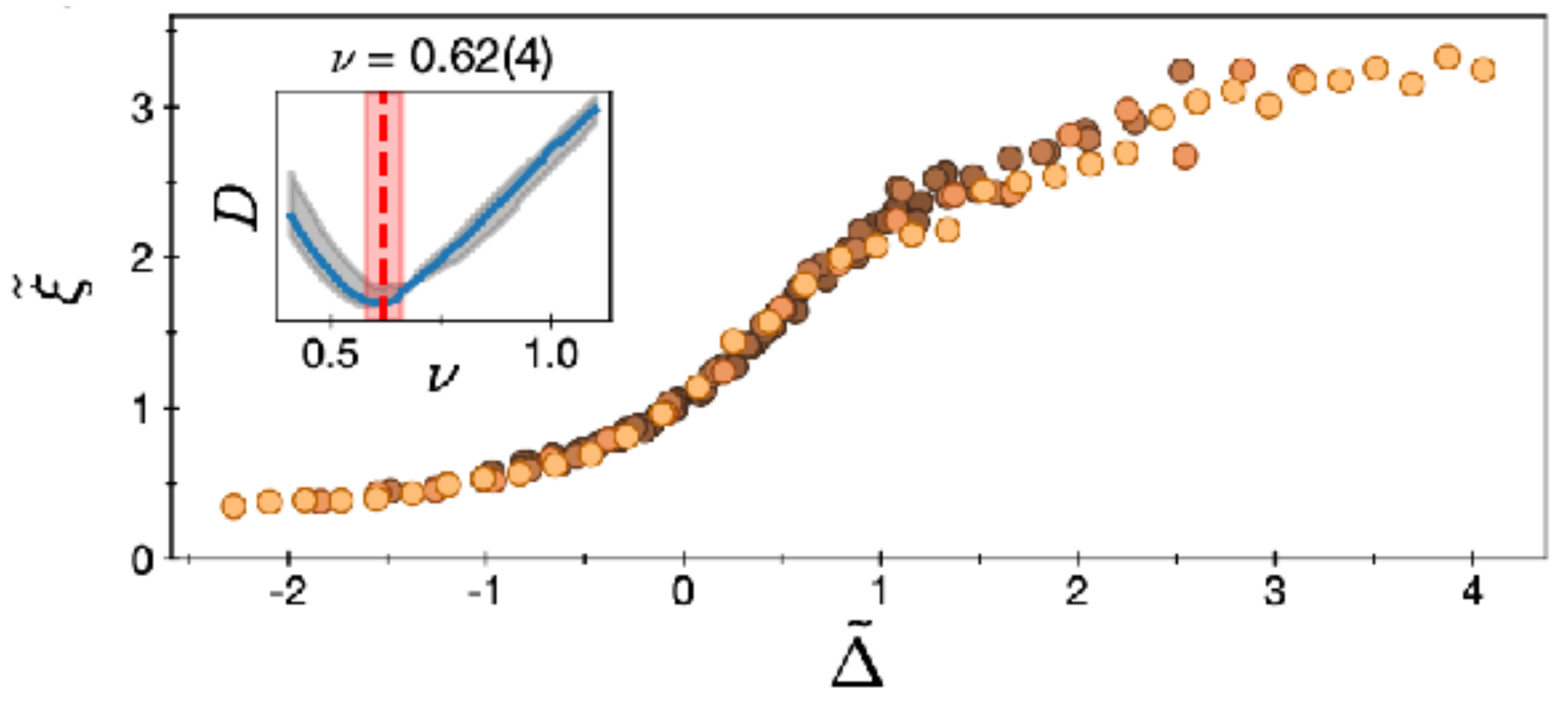
2*D*: Quantum critical points

Samajdar, Ho, Pichler, Lukin, Sachdev,
Phys. Rev. Lett. 124, 103601 (2020)



Ebadi et. al. arXiv:2012.12281
Nature 595, 227 (2021)





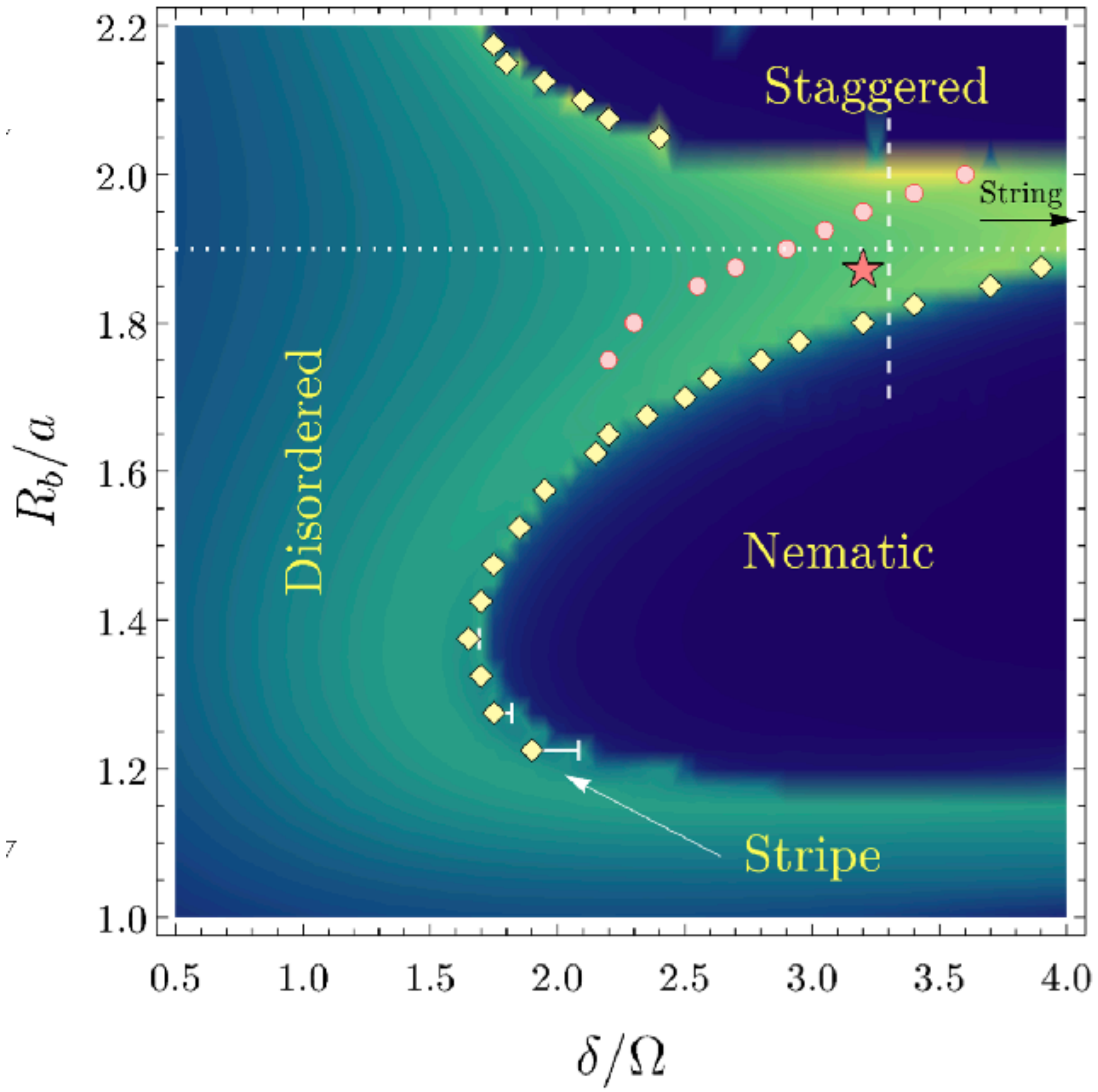
- First experimental realization of a 2+1 D QCP in the Ising universality class

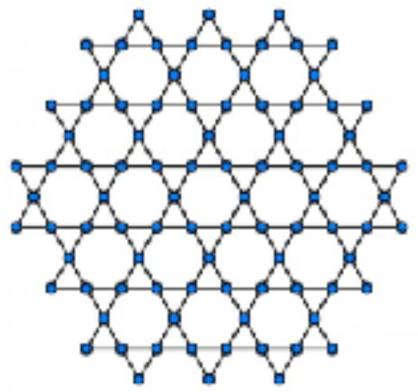
2*D*: Quantum spin liquids

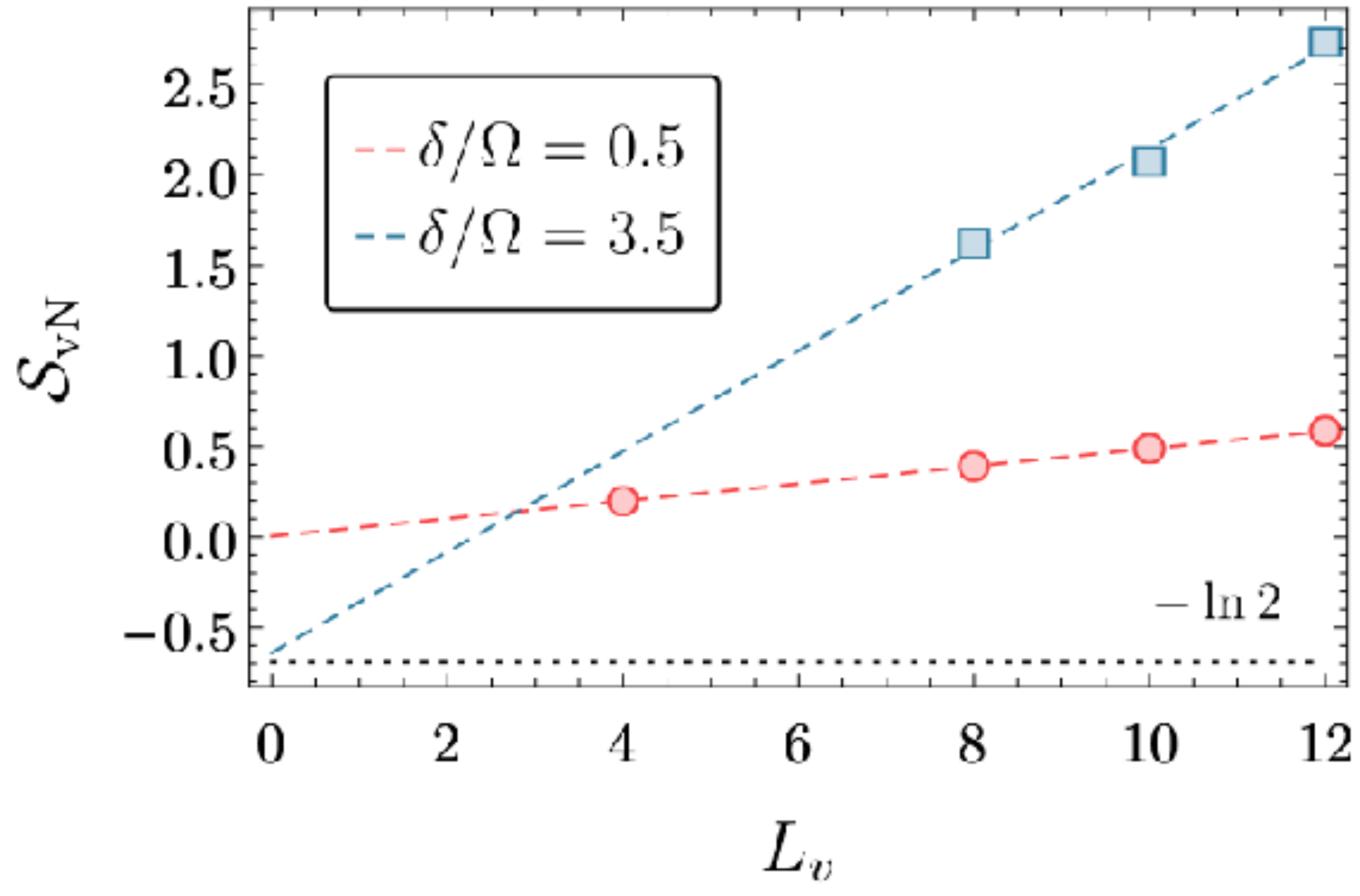
$$S = aL - \ln(2)$$

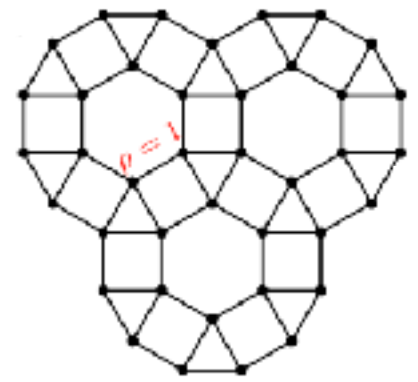
Signature of a Z2 spin liquid S_{topo}

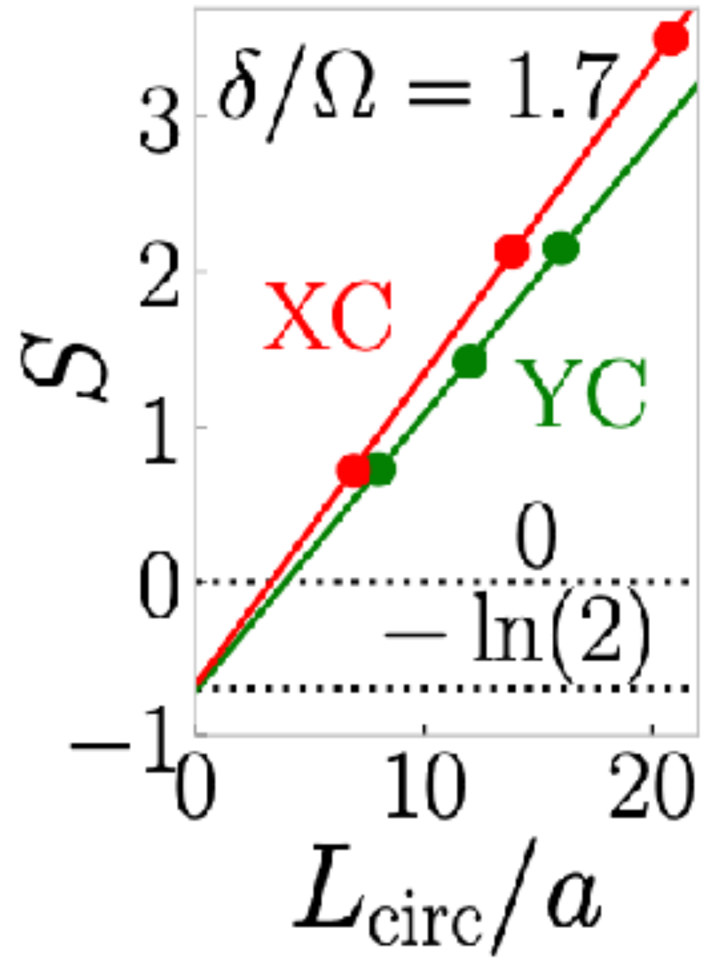
Samajdar, Ho, Pichler, Lukin, Sachdev, Proc. Natl. Acad. Sci. 118 (2021)
Verresen, Lukin, Vishwanath, Phys. Rev. X 11, 031005 (2021)



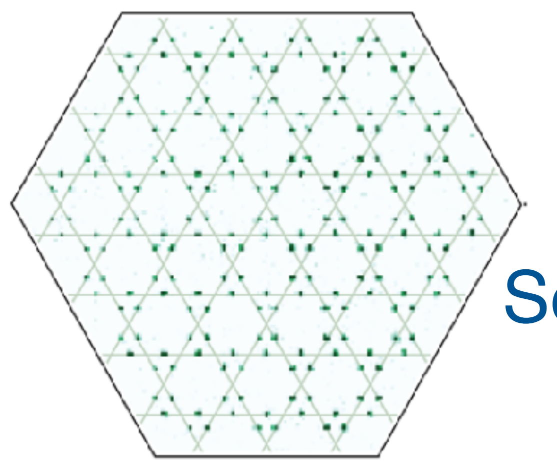








- Motivating experimental searches



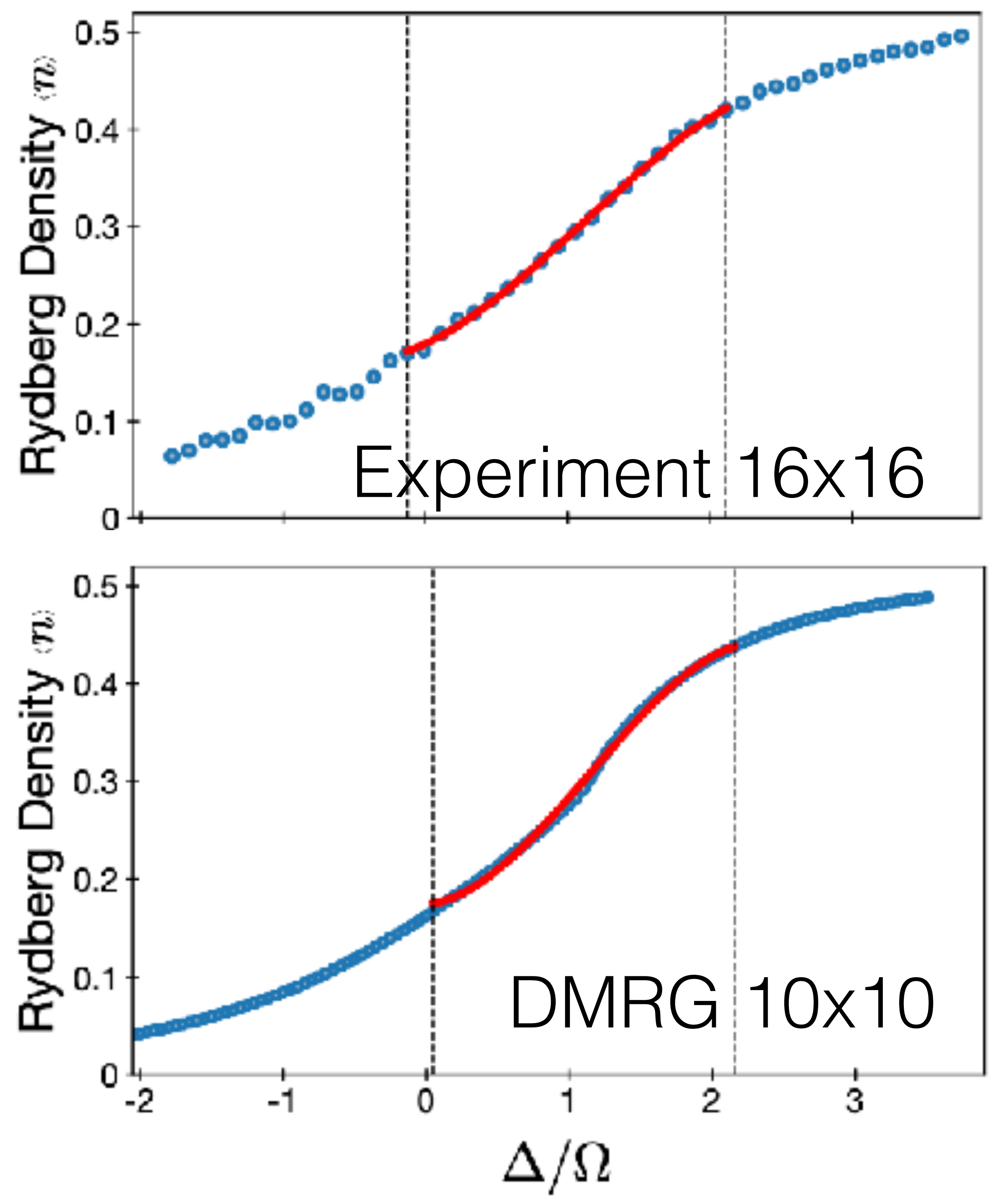
Semeghini et. al. arXiv:2104.04119
(219 atoms)

Outline

- Rydberg array quantum simulators/emulators
- *In silico* simulation strategies: DMRG, QMC
- Data-driven strategies: neural network wavefunctions & VMC

in silico simulation strategies: DMRG/MPS

Ebadi et. al. Nature 595, 227 (2021)



Quantum simulation of 2D antiferromagnets with hundreds of Rydberg atoms

Pascal Scholl, Michael Schuler, Hannah J. Williams, Alexander A. Eberharter, Daniel Barredo, Kai-Niklas Schymik, Vincent Lienhard, Louis-Paul Henry, Thomas C. Lang, Thierry Lahaye, Andreas M. Läuchli & Antoine Browaeys

Nature **595**, 233–238 (2021)

"MPS simulations for systems up to ***L = 10*** are reliable to characterize and benchmark the experimental results, although they might not be fully converged in χ with regard to other observables, such as the entanglement entropy. Finally, we want to mention that reliable simulations of the dynamics for the largest experimental results achieved in this paper (***L = 14***) seem to be out of reach with currently available computational hardware…"

- DMRG/MPS is currently the standard for comparison with experiment
- Enabled by open source libraries such as iTensor and TeNPy

in silico simulation strategies: QMC

Note: the Rydberg Hamiltonian is (efficiently made) stoquastic

$$H = \Omega \sum_i \sigma_i^x - \Delta \sum_i n_i + \sum_{i<j} V_{ij} n_i n_j$$

$$H = \begin{pmatrix} d & -|o| & -|o| & -|o| & -|o| \\ -|o| & d & -|o| & -|o| & -|o| \\ -|o| & -|o| & d & -|o| & -|o| \\ -|o| & -|o| & -|o| & d & -|o| \\ -|o| & -|o| & -|o| & -|o| & d \end{pmatrix}$$

- Allows for (efficient?) simulation by quantum Monte Carlo

$$Z = \mathrm{Tr}\left\{e^{-\beta \hat{H}}\right\} = \sum_{\alpha_0} \langle \alpha_0 | \sum_{n=0}^{\infty} \frac{\beta^n}{n!} (-\hat{H})^n | \alpha_0 \rangle \qquad Z \equiv \langle \psi_0 | \psi_0 \rangle = \langle \alpha_\ell | (-\hat{H})^M (-\hat{H})^M | \alpha_r \rangle$$

- Perron-Frobenius guarantees a real/positive groundstate wavefunction

$$\psi_\lambda(\mathbf{x}) = \sqrt{p_\lambda(\mathbf{x})}$$

Efficient QMC: sign-free and ergodic

Stochastic series expansion

$$\hat{H} = \frac{\Omega}{2}\sum_{i=1}^{N}\hat{\sigma}_i^x - \delta\sum_{i=1}^{N}\hat{n}_i + \sum_{i<j}V_{ij}\hat{n}_i\hat{n}_j$$

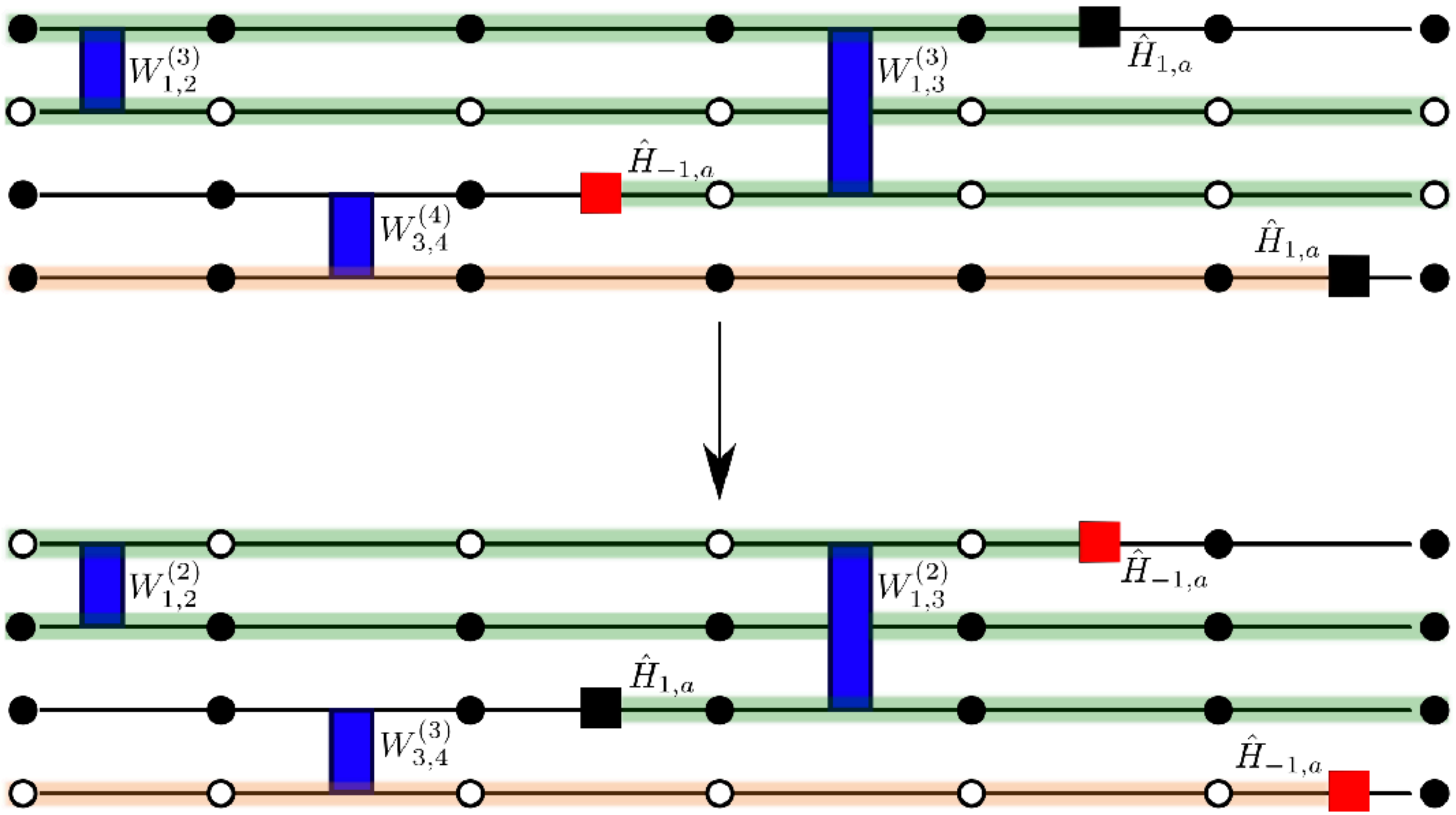
Sandvik, Phys. Rev. E 68(5), 056701 (2003)
Merali, De Vlugt, RGM, arXiv:2107.00766
(c.f. Kalinowski *et al.* arXiv:2112.10790)

$$\langle 1|\hat{H}_{-1,a}|0\rangle = \langle 0|\hat{H}_{-1,a}|1\rangle = \frac{\Omega}{2},$$
$$\langle 1|\hat{H}_{1,a}|1\rangle = \langle 0|\hat{H}_{1,a}|0\rangle = \frac{\Omega}{2},$$
$$W_{ij}^{(1)} \equiv \langle 00|\hat{H}_{1,b}|00\rangle = C_{ij},$$
$$W_{ij}^{(2)} \equiv \langle 01|\hat{H}_{1,b}|01\rangle = \delta_b + C_{ij},$$
$$W_{ij}^{(3)} \equiv \langle 10|\hat{H}_{1,b}|10\rangle = \delta_b + C_{ij},$$
$$W_{ij}^{(4)} \equiv \langle 11|\hat{H}_{1,b}|11\rangle = -V_{ij} + 2\delta_b + C_{ij}$$

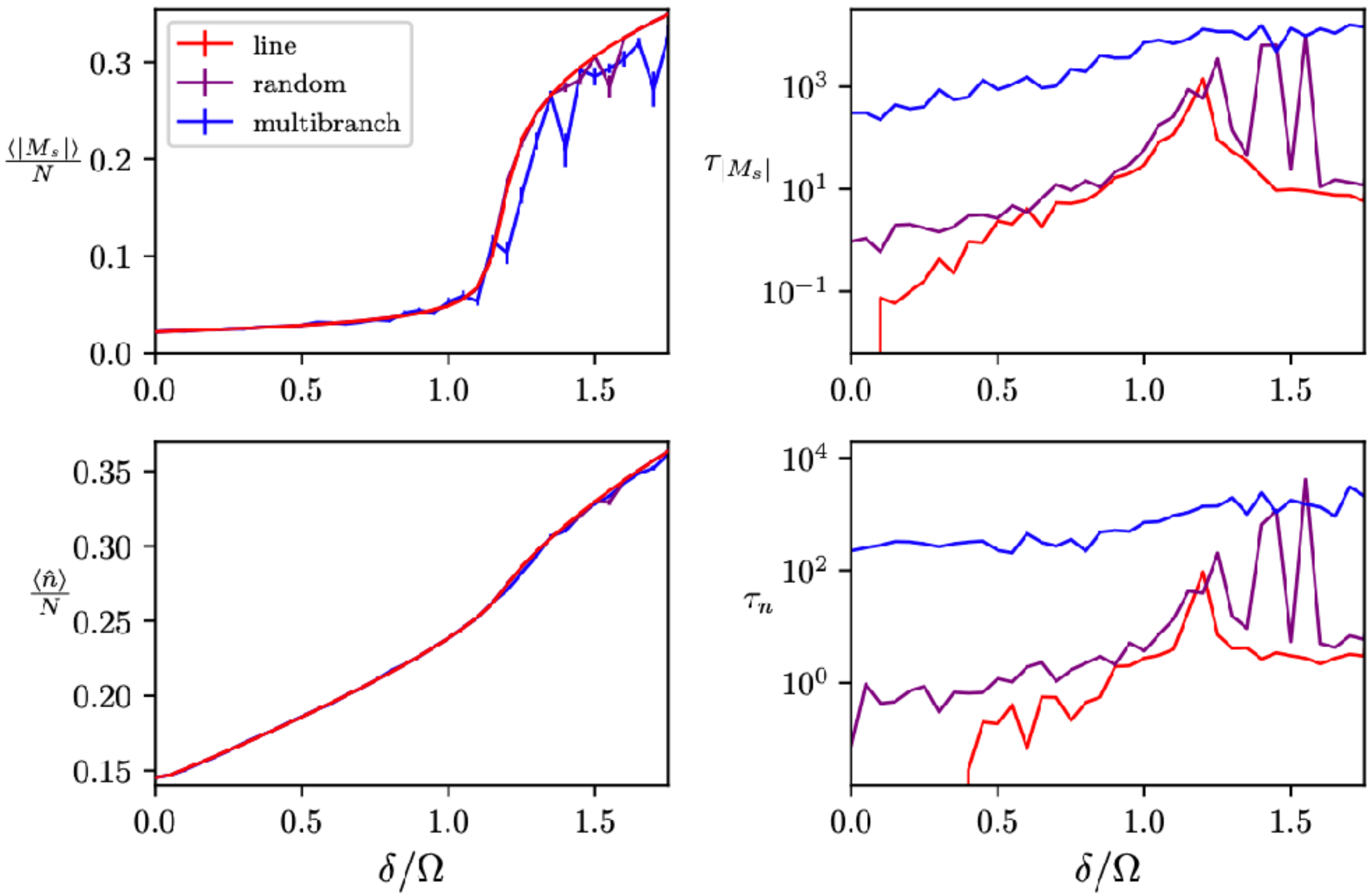
$$\delta_b = \delta/(N-1)$$

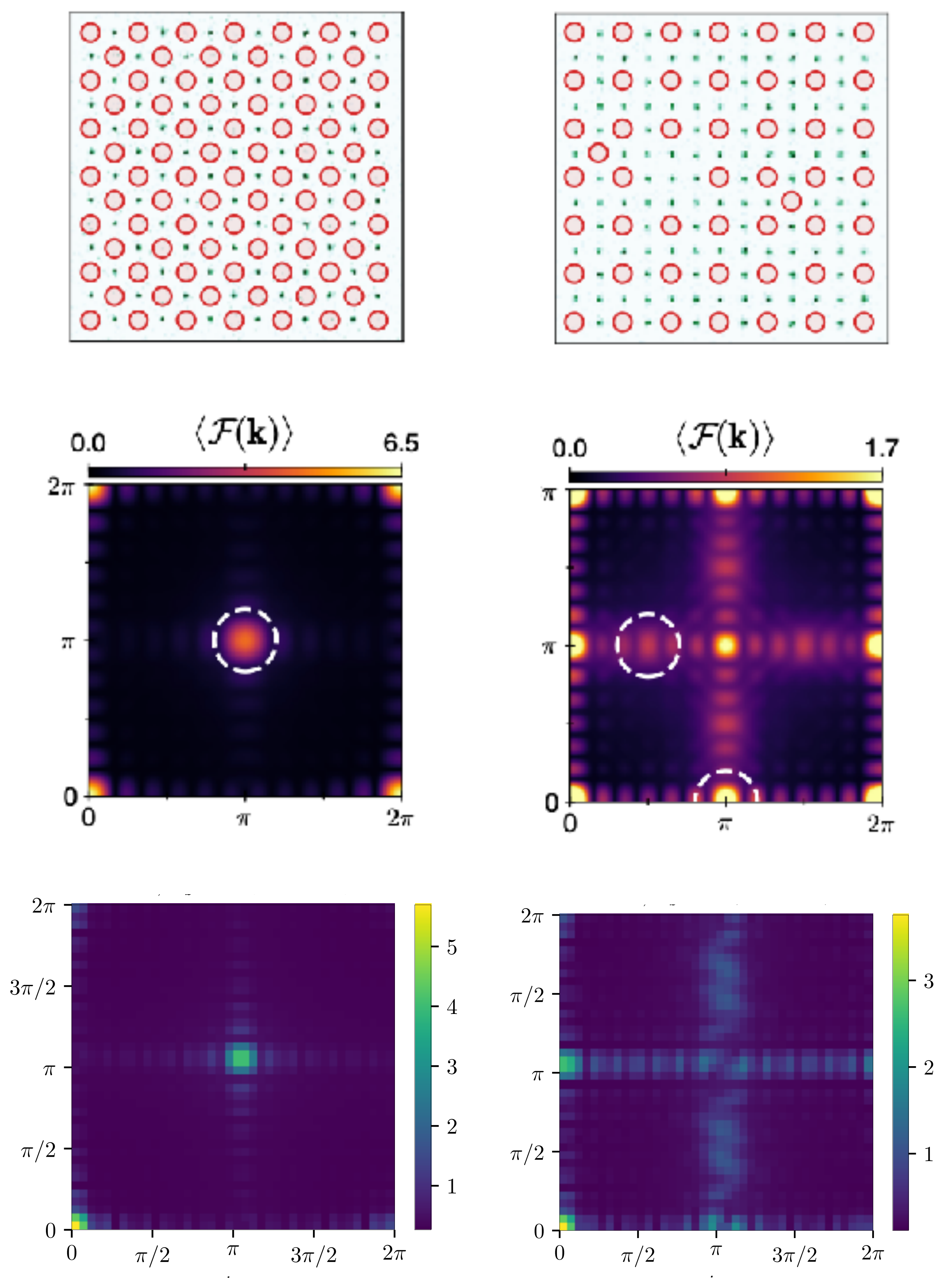
$$C_{ij} = |\min(0, \delta_b, 2\delta_b - V_{ij})|$$

$$Z \equiv \langle\psi_0|\psi_0\rangle = \langle\alpha_\ell|(-\hat{H})^M(-\hat{H})^M|\alpha_r\rangle$$



Efficient QMC: sign-free and ergodic





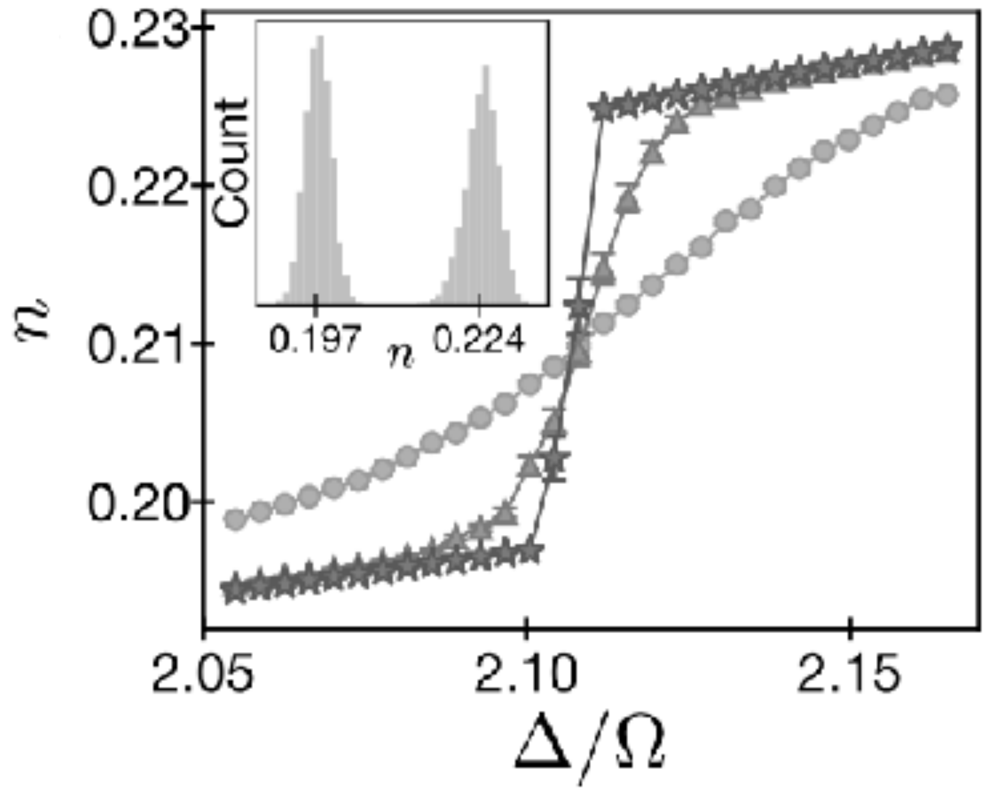
Merali, De Vlugt, RGM, arXiv:2107.00766
S. Czischek *et al.*

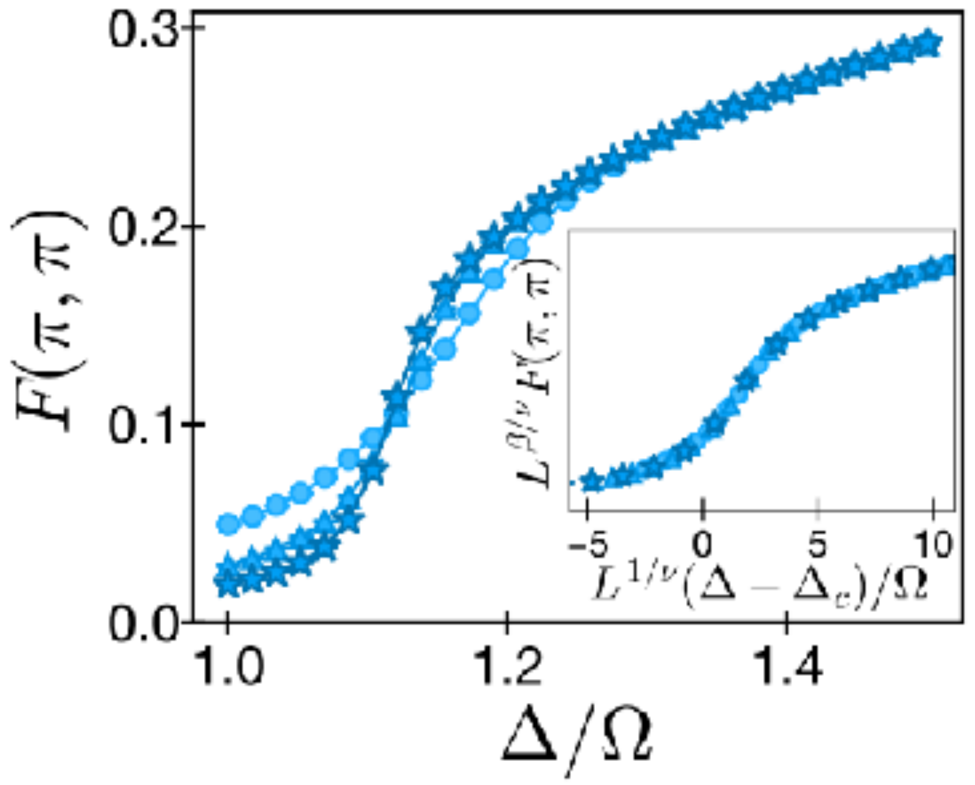
- Detailed comparisons with experiment are possible
- Autocorrelation times can be very significant
- Not clear what the maximum lattice sizes are at this time

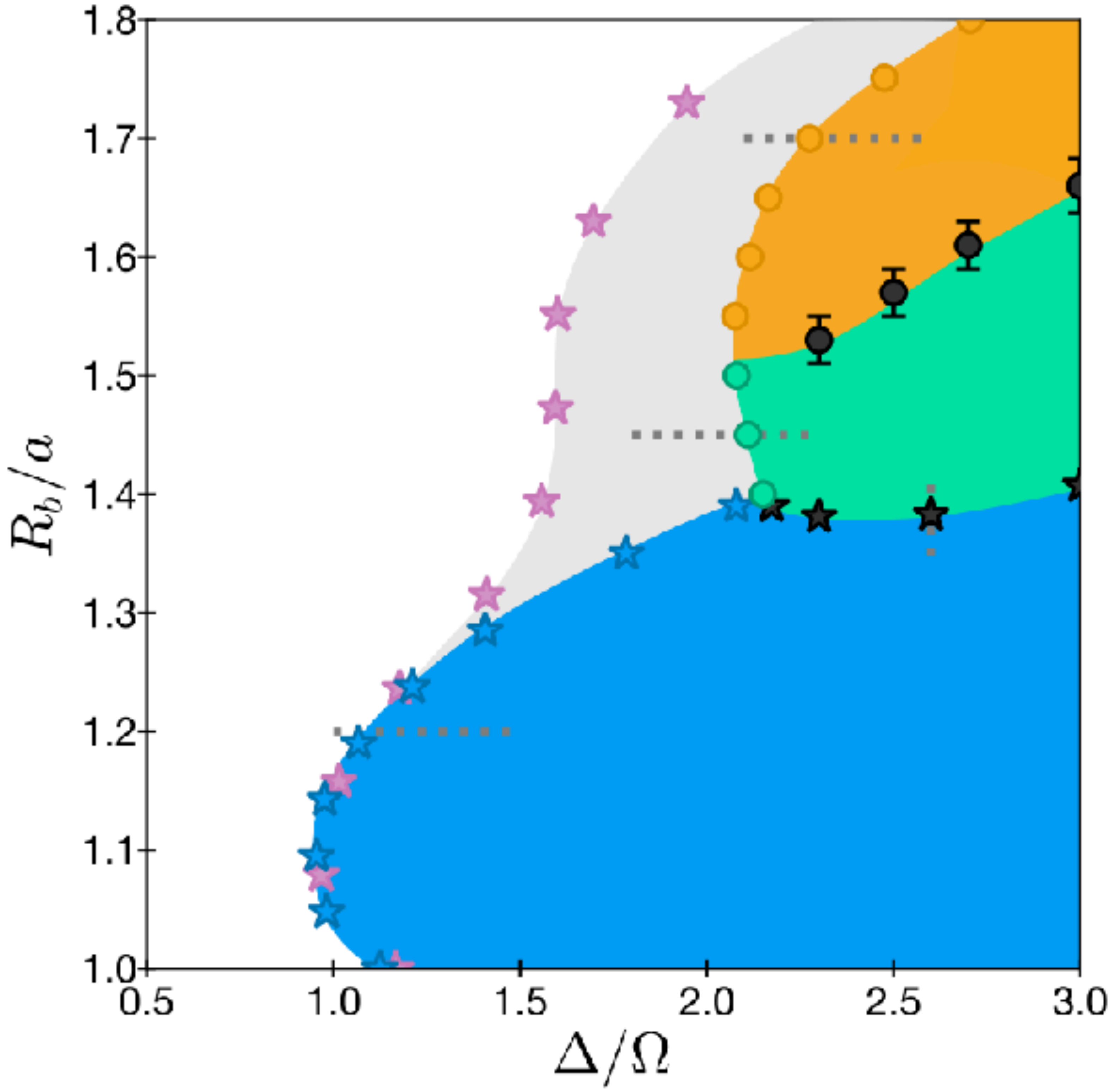
Continuous imaginary time QMC

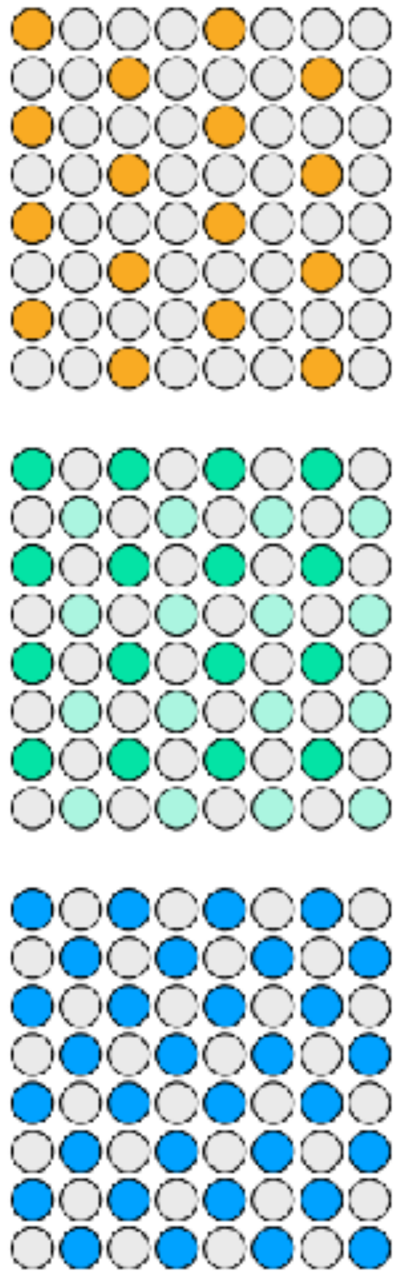
Bulk and Boundary Quantum Phase Transitions in a Square Rydberg Atom Array
M. Kalinowski, R. Samajdar, RGM, M. Lukin, S. Sachdev, S. Choi, arXiv:2112.10790

$L = 8$
$L = 12$
$L = 16$









- Clear differences between OBC and PBC systems - boundary plays major role
- Consequences for adiabatic state preparation, optimization problems

Outline

- Rydberg array quantum simulators/emulators
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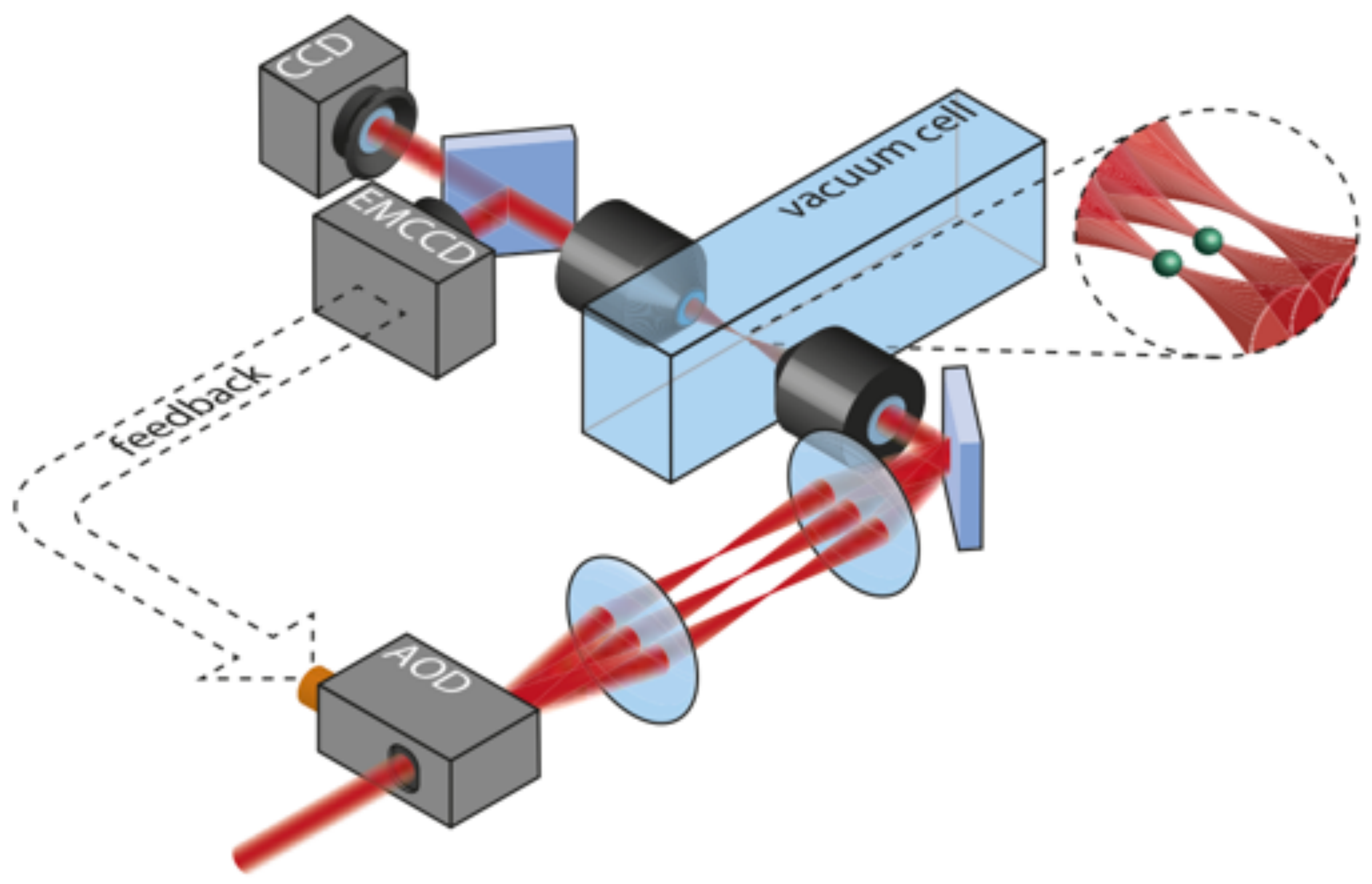
Data driven state reconstruction

The availability of high quality projective measurement data allows for state reconstruction, e.g. through the KL divergence or maximum likelihood methods



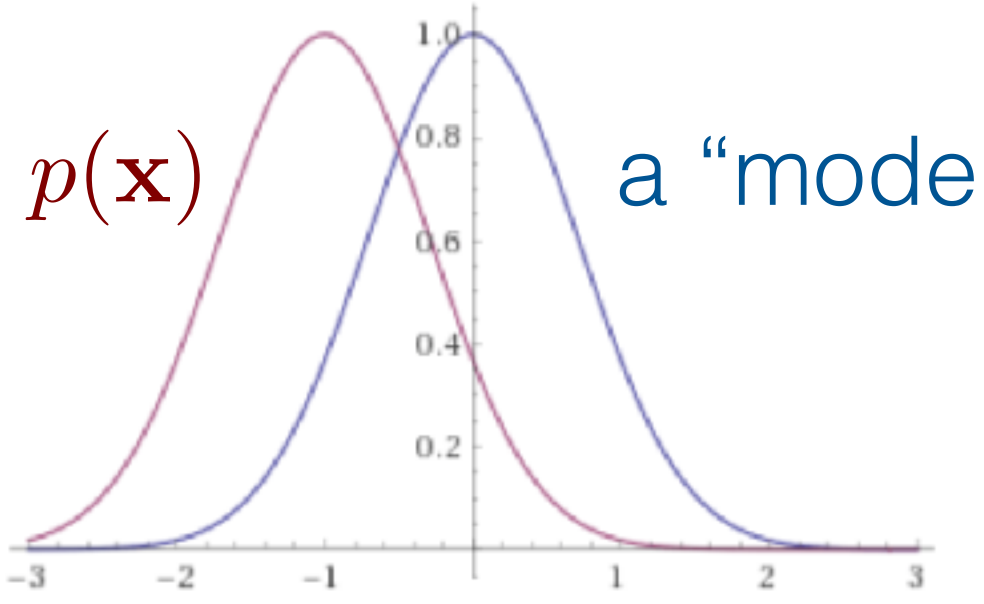
qubit projective measurement data distributed according to Born rule, $p(\mathbf{x})$

$$\left.\begin{aligned}
\mathbf{x}_1 &= (1,0,0,1,1,1,0,0,0,0,\cdots,1)\\
\mathbf{x}_2 &= (1,1,1,0,1,1,0,1,1,1,\cdots,1)\\
\mathbf{x}_3 &= (0,1,1,0,0,1,0,1,0,1,\cdots,0)\\
&\vdots
\end{aligned}\right\}\mathcal{D}$$

Cost function:

$$\mathrm{KL}(p||p_\lambda) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{p_\lambda(\mathbf{x})} \geq 0$$

$p(\mathbf{x})$

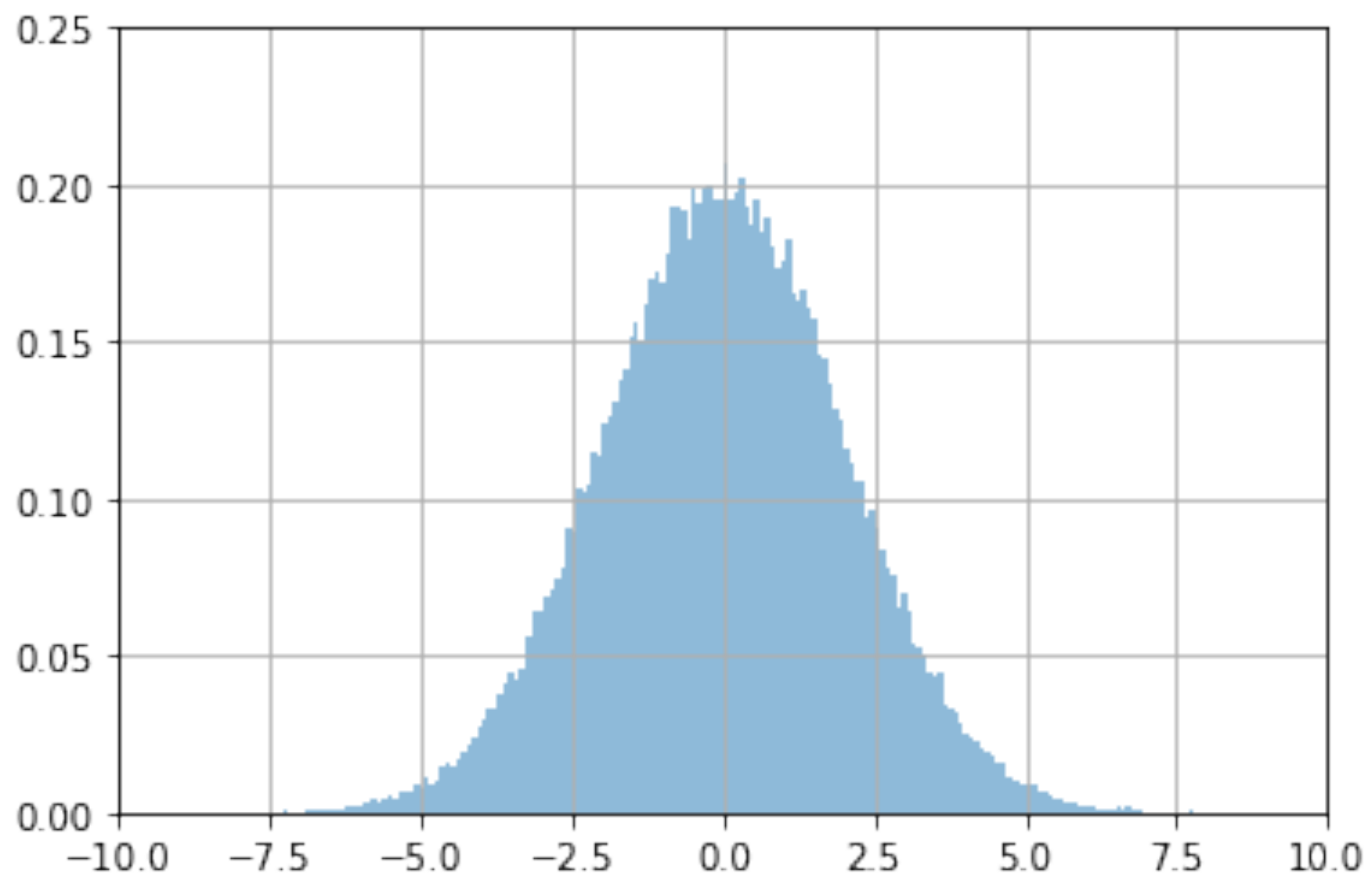


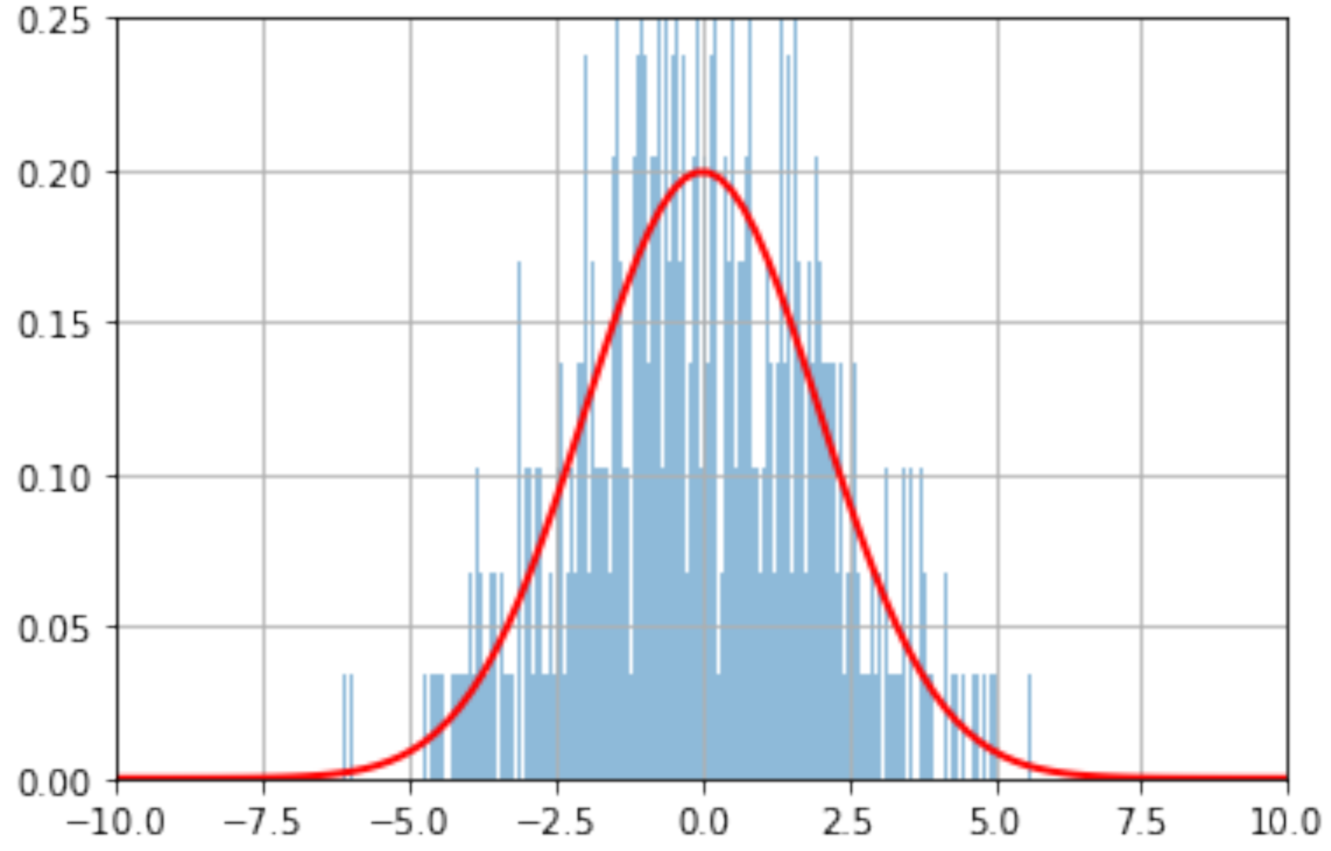
a “model” $p_\lambda(\mathbf{x})$

Parameterized models and generalization

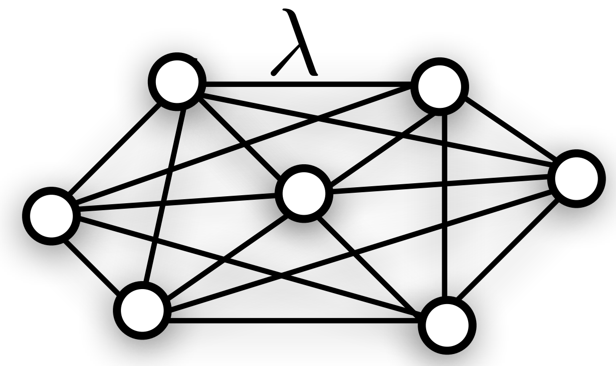
- Rydberg data is limited by the experimental shot budget (~3/s)
- *Generative models* use inductive bias (assumptions in the model) in order to help generalize to unseen data

$$p(x) \approx \frac{1}{||\mathcal{D}||} \sum_{\mathbf{x}_k \in \mathcal{D}} \delta_{\mathbf{x},\mathbf{x}_k}$$

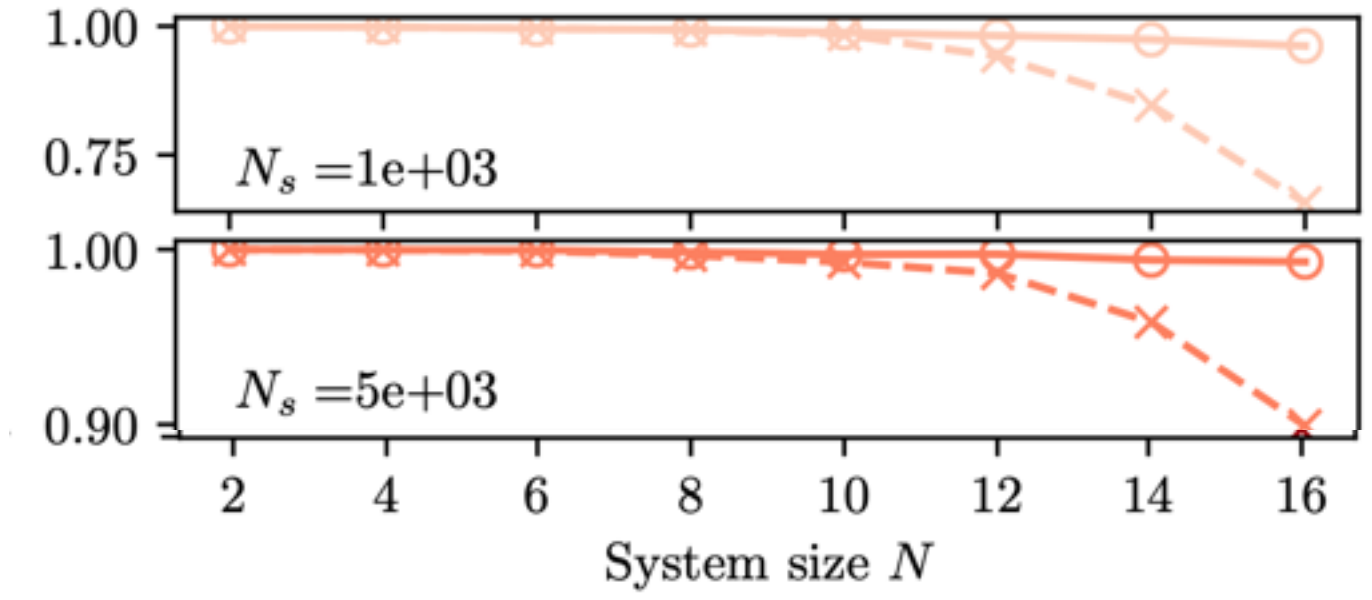




$$p_\lambda(x) \approx$$



Fidelity improvements for RBMs vs. frequency-distribution reconstructions, for a selection of dataset sizes Ns.

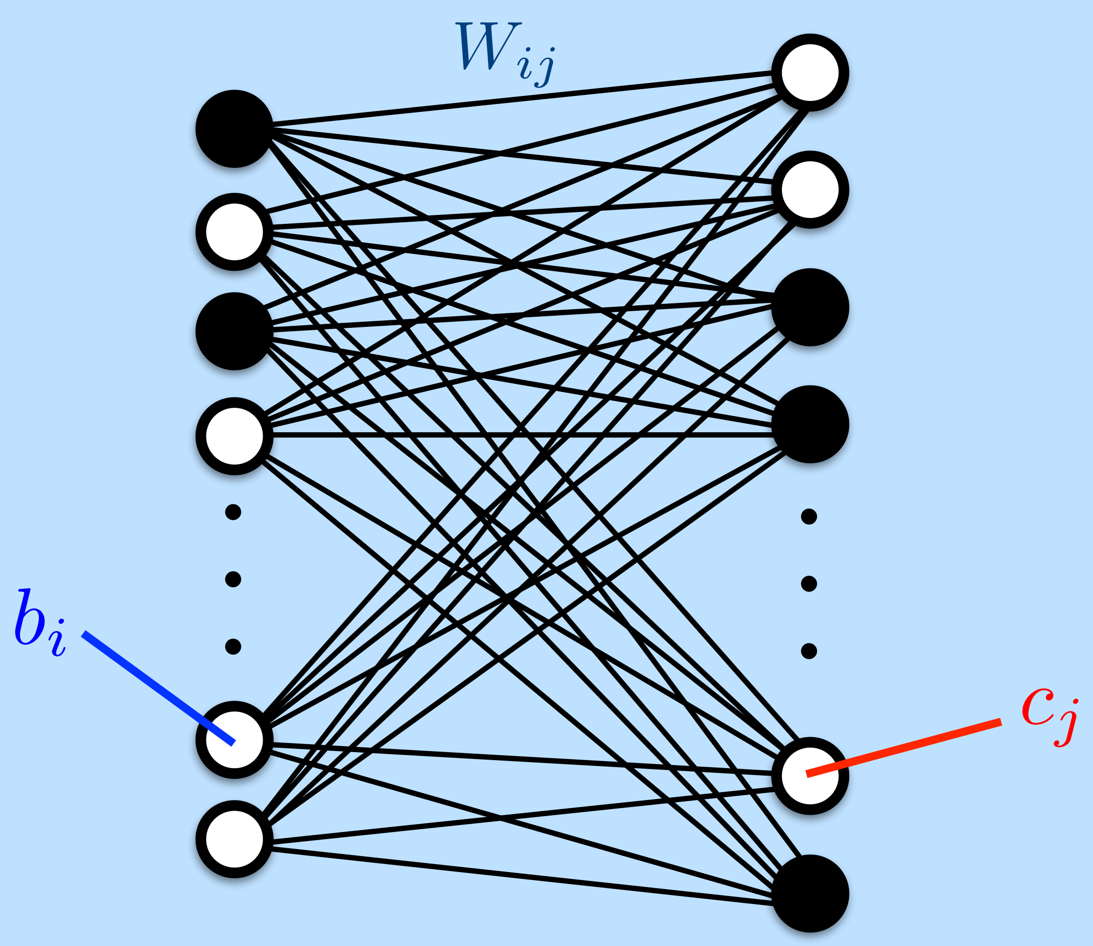


B. Timar

Neural network wavefunctions

Torlai and RGM, Phys. Rev. B 94, 165134 (2016); Carleo, Troyer Science 355, 602 (2017)
Hibat-Allah, Ganahl, Hayward, RGM, and Carrasquilla, Phys. Rev. Research 2, 023358 (2020)

Restricted Boltzmann Machine



$$p_\lambda = \frac{1}{Z_\lambda} e^{-E_\lambda(\mathbf{x},\mathbf{h})}$$

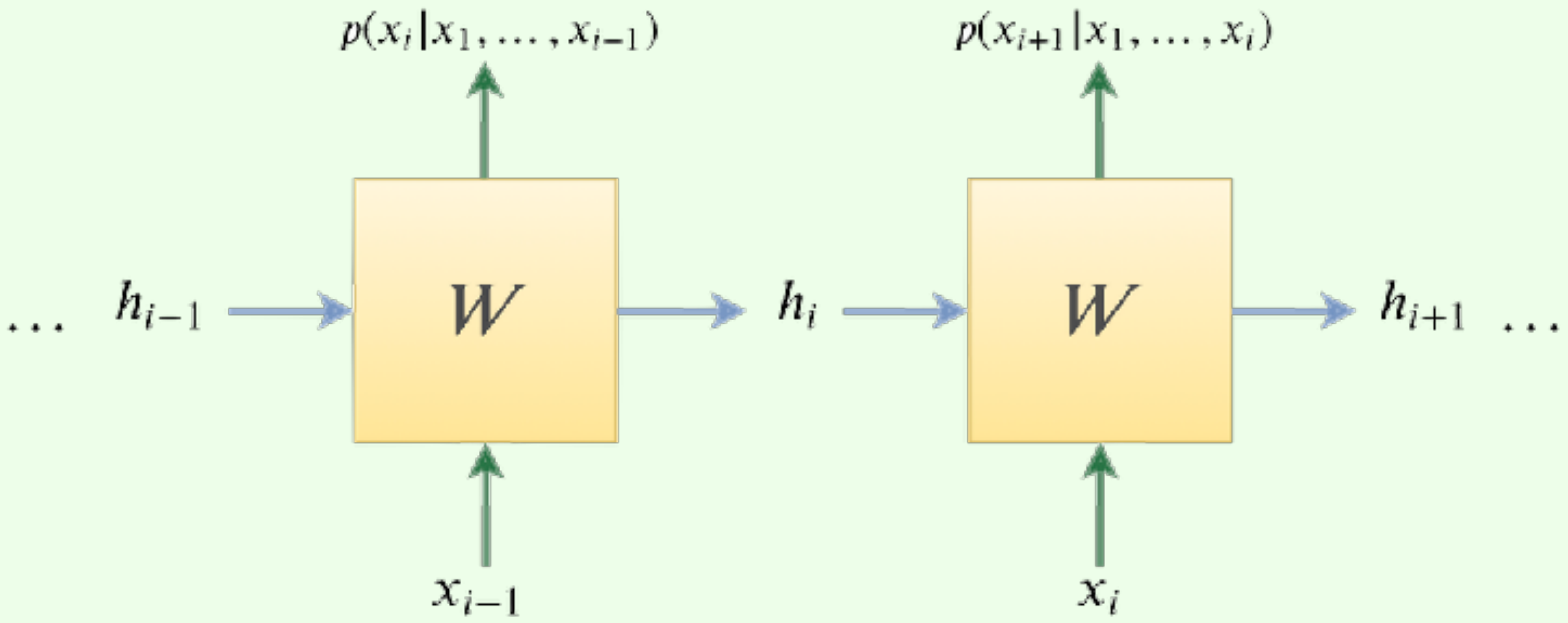
$$p_\lambda(\mathbf{x}) = \sum_{\mathbf{h}} p_\lambda(\mathbf{x},\mathbf{h})$$

$x_i = 0,1$ $\quad$ $h_j = 0,1$

$$E_\lambda(\mathbf{x},\mathbf{h}) = -\sum_{ij} W_{ij} x_i h_j - \sum_i b_i x_i - \sum_j c_j h_j$$

$\lambda = \{W, b, c\}$ model parameters

Recurrent Neural Network

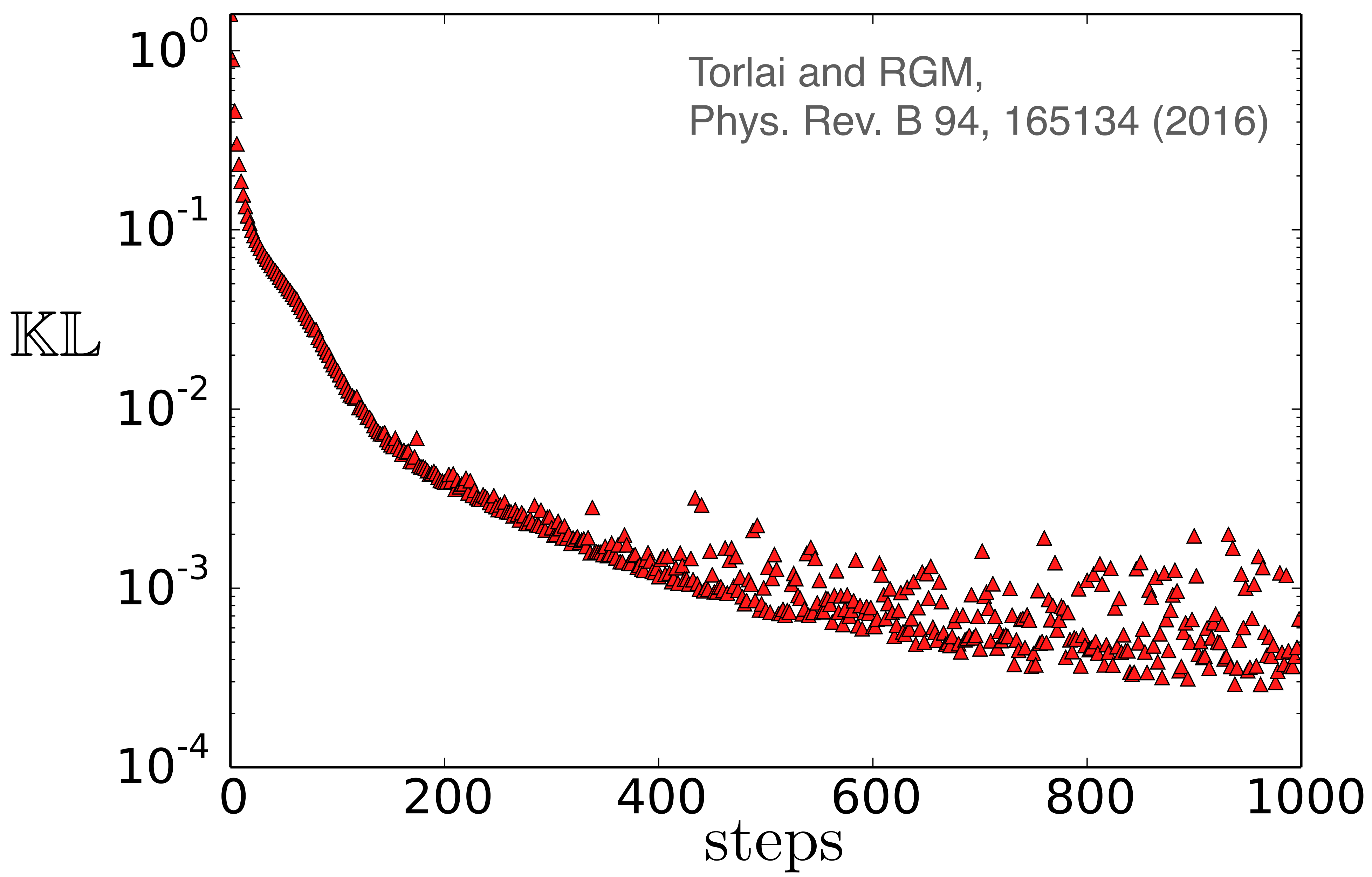


$$p_\lambda(x_1,\cdots x_N) = \prod_{i=1}^{N} p(x_i|x_1,\ldots,x_{i-1})$$

$$= p(x_1)p(x_2|x_1)p(x_3|x_1,x_2)\cdots$$

Autoregressive model; produces independent samples

Training & sampling



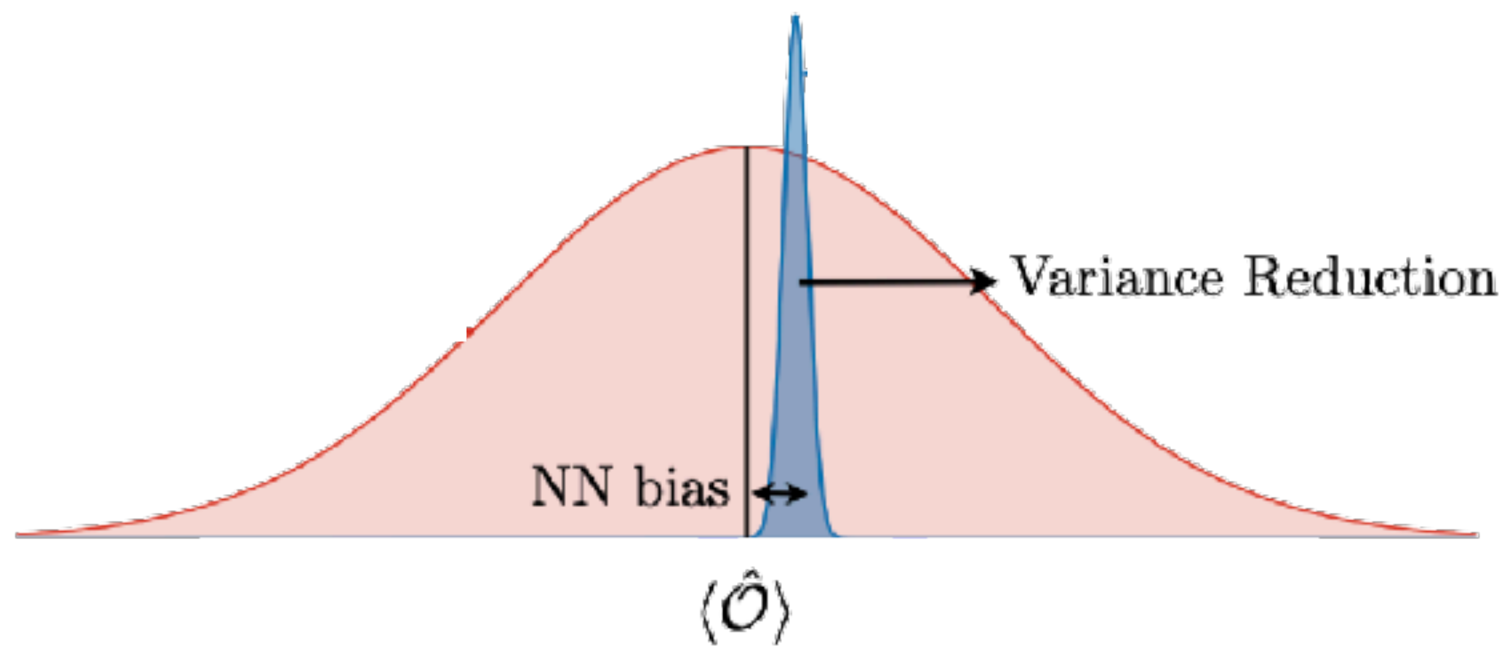
Training: stochastic gradient descent:

$$\lambda' = \lambda - \eta \nabla \mathrm{KL}$$

$$\mathrm{KL}(p||p_\lambda) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{p_\lambda(\mathbf{x})} \geq 0 \qquad \mathcal{L} = \langle \log p_\lambda(\mathbf{x}) \rangle_p$$

Rydberg Hamiltonian: occupation basis is informationally complete $\quad \psi_\lambda(\mathbf{x}) = \sqrt{p_\lambda(\mathbf{x})}$

Can reconstruct estimators by sampling the trained model $\quad \langle A^{\mathrm{D}} \rangle = \sum_{\mathbf{x}} p_\lambda(\mathbf{x}) A_{\mathbf{x}}$



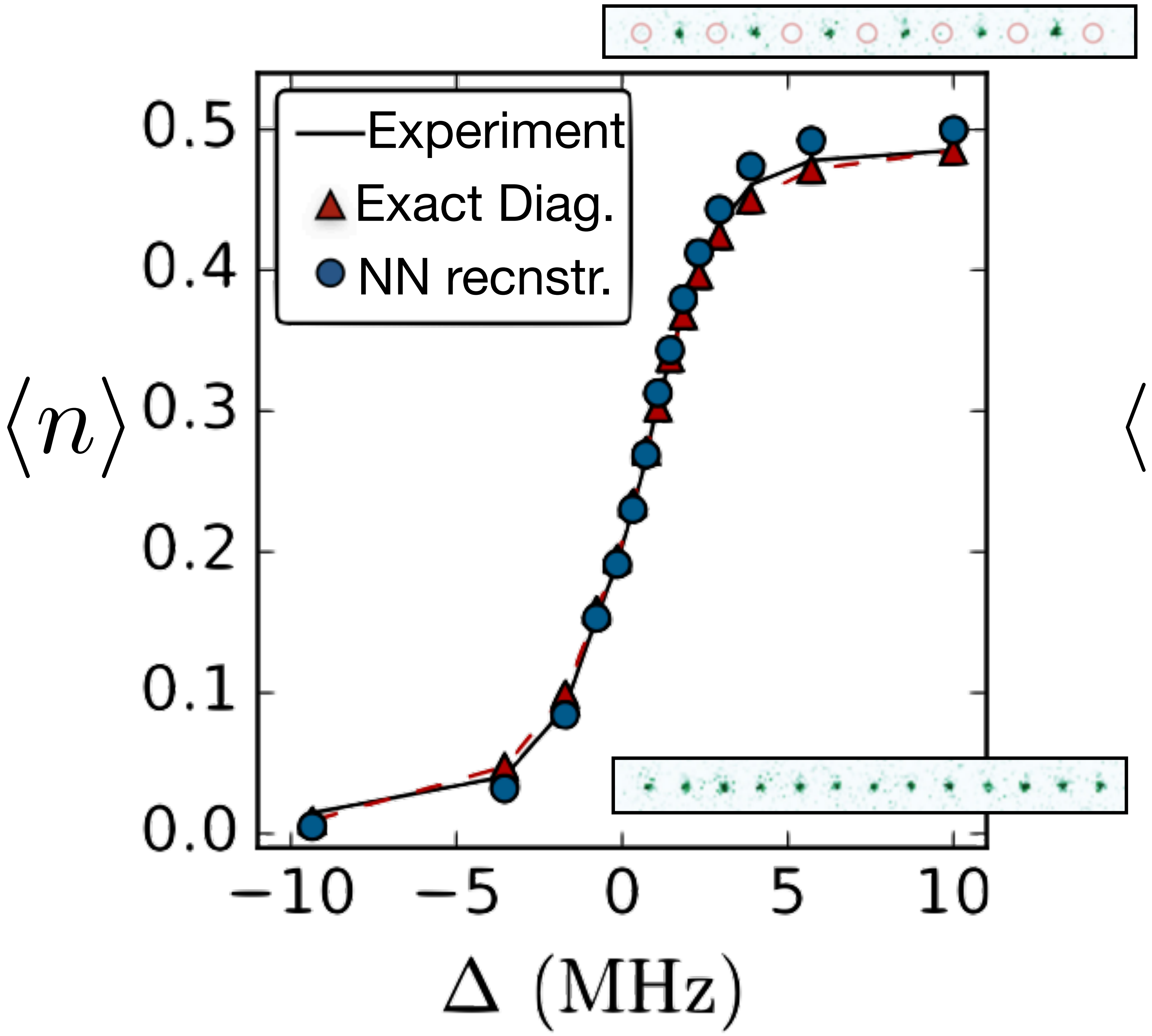
Bias-variance tradeoff

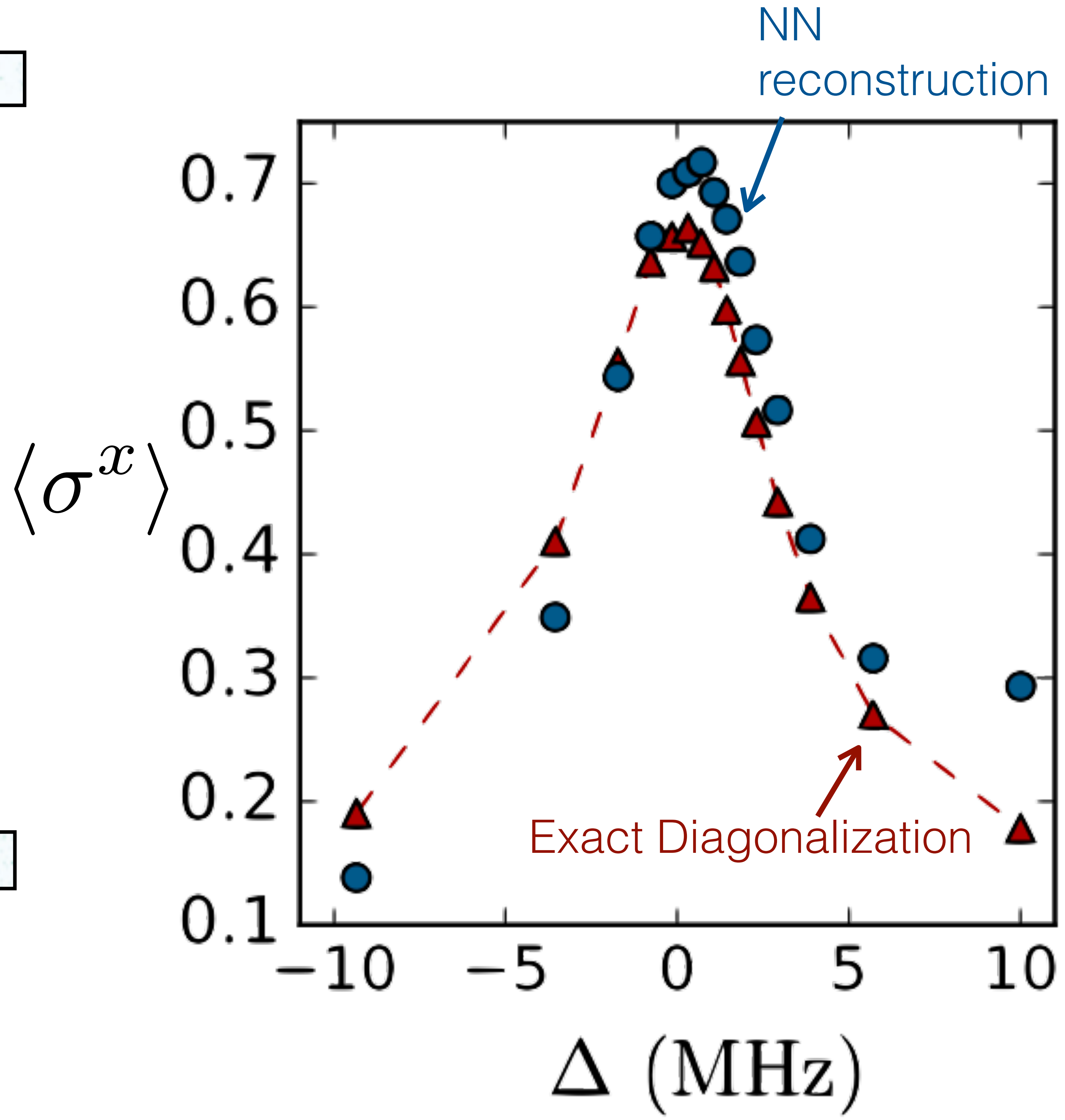
Torlai, Mazzola, Carleo, and Mezzacapo Phys. Rev. Research 2, 022060 (2020)

Rydberg state reconstruction

Torlai, Timar, van Nieuwenburg, Levine, Omran, Keesling, Bernien, Greiner, Vuletić, Lukin, RGM, Endres, Phys. Rev. Lett. 123, 230504 (2019)

- one-dimensional chain
- 3000 projective measurements per detuning parameter
- assume positively & purity of the state - use RBM





Stoquastic Hamiltonian:

$$\psi_\lambda(z) = \sqrt{p_\lambda(z)}$$

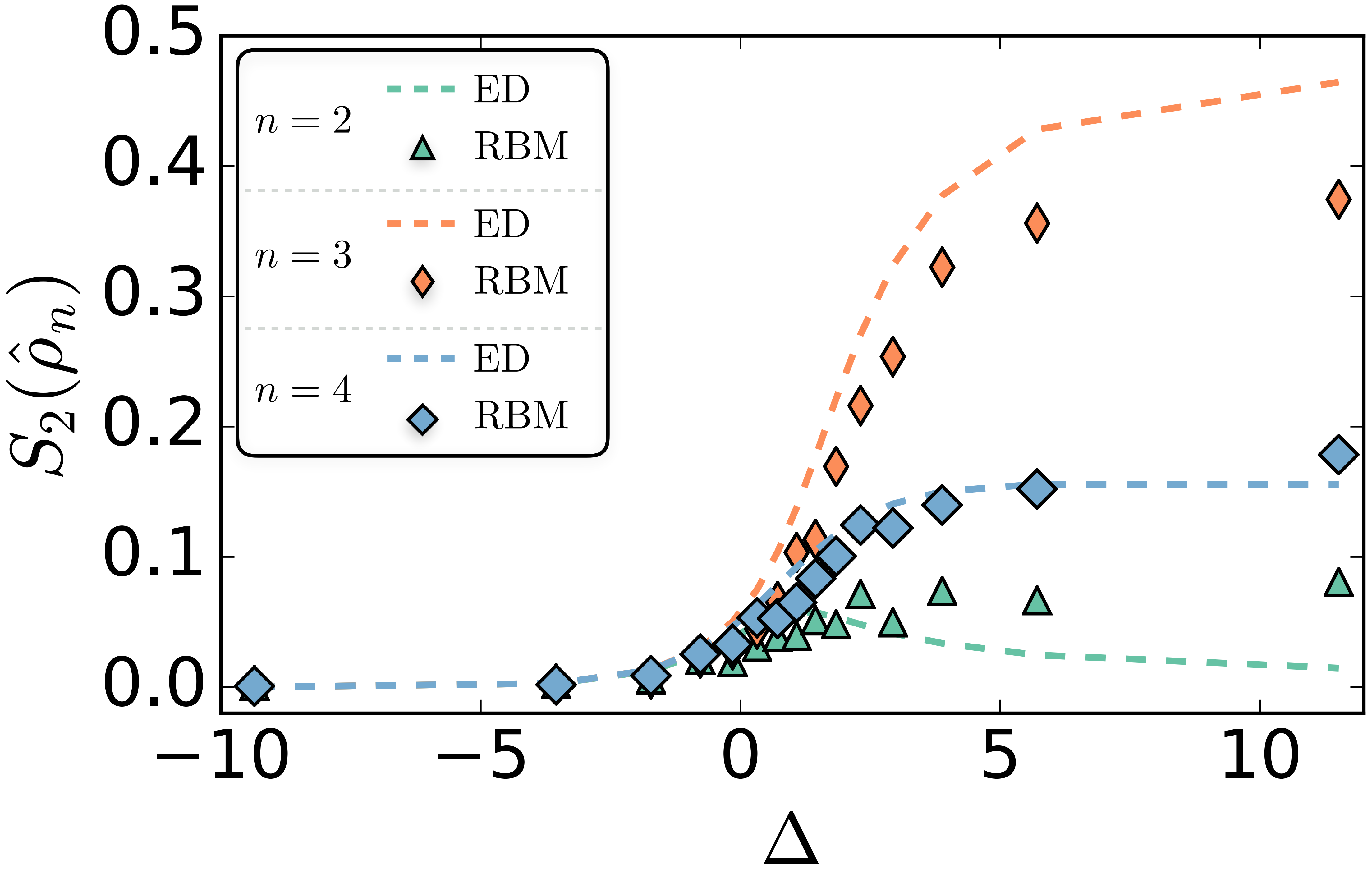
$$\langle \mathcal{O} \rangle = \sum_{zz'} \psi_\lambda(z)\psi_\lambda(z')\mathcal{O}_{zz'}$$

$$= \sum_{z} \psi_\lambda^2(z) \boxed{\sum_{z'} \frac{\psi_\lambda(z')}{\psi_\lambda(z)} \mathcal{O}_{zz'}}$$

"local" estimator

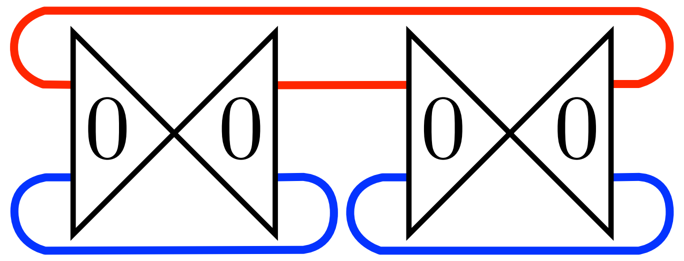
Experimental reconstruction

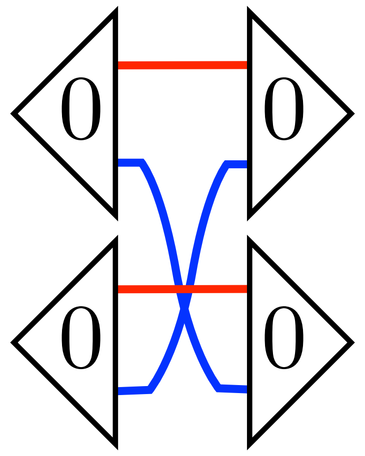
- Second Renyi entropy via SWAP



$$S_2(\rho_A) = -\log\left[\mathrm{Tr}(\rho_A^2)\right]$$

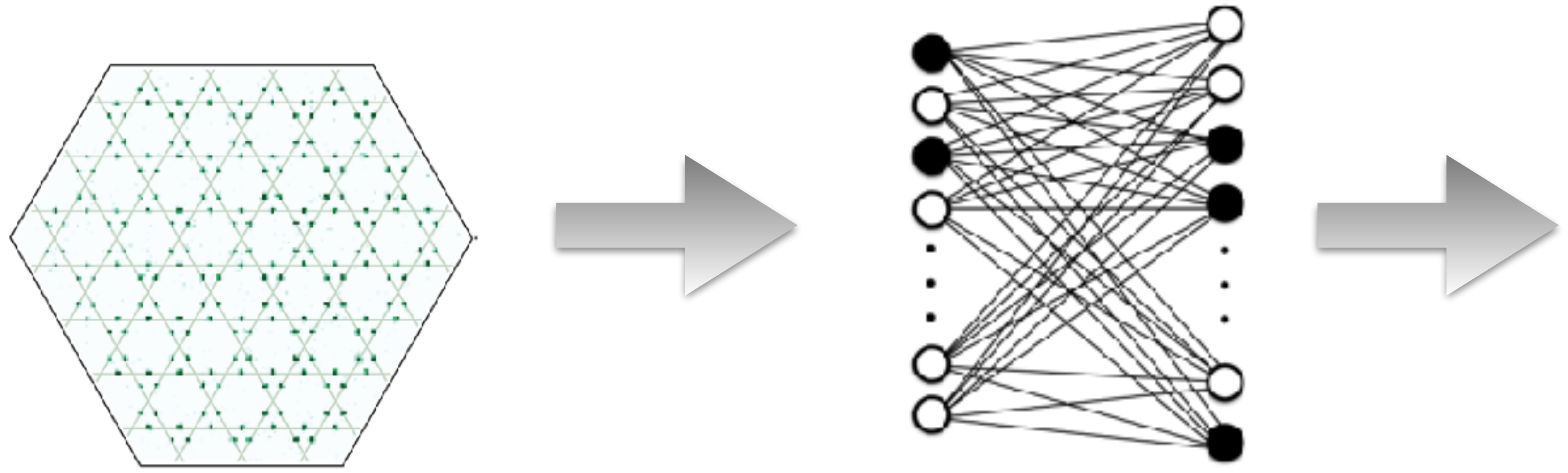
$\mathrm{Tr}(\rho_{\mathrm{A}}^2) \Leftrightarrow$

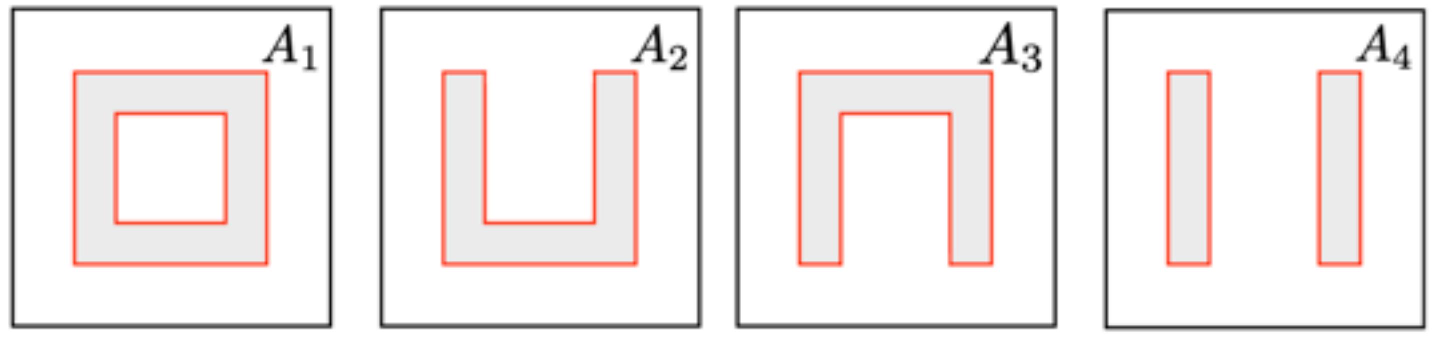




$\Leftrightarrow \langle Swap_{\mathrm{B}} \rangle$

- With more data…

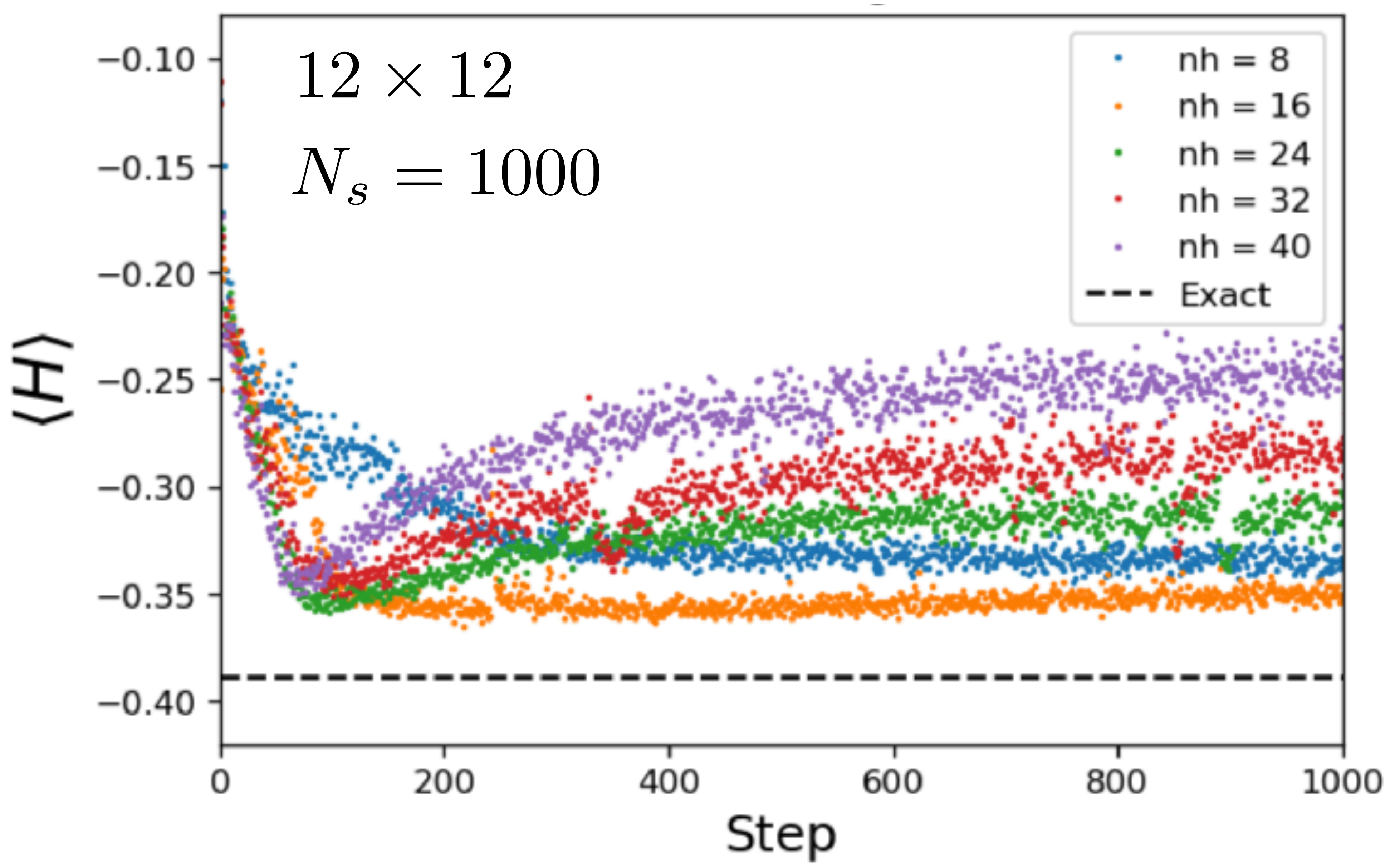


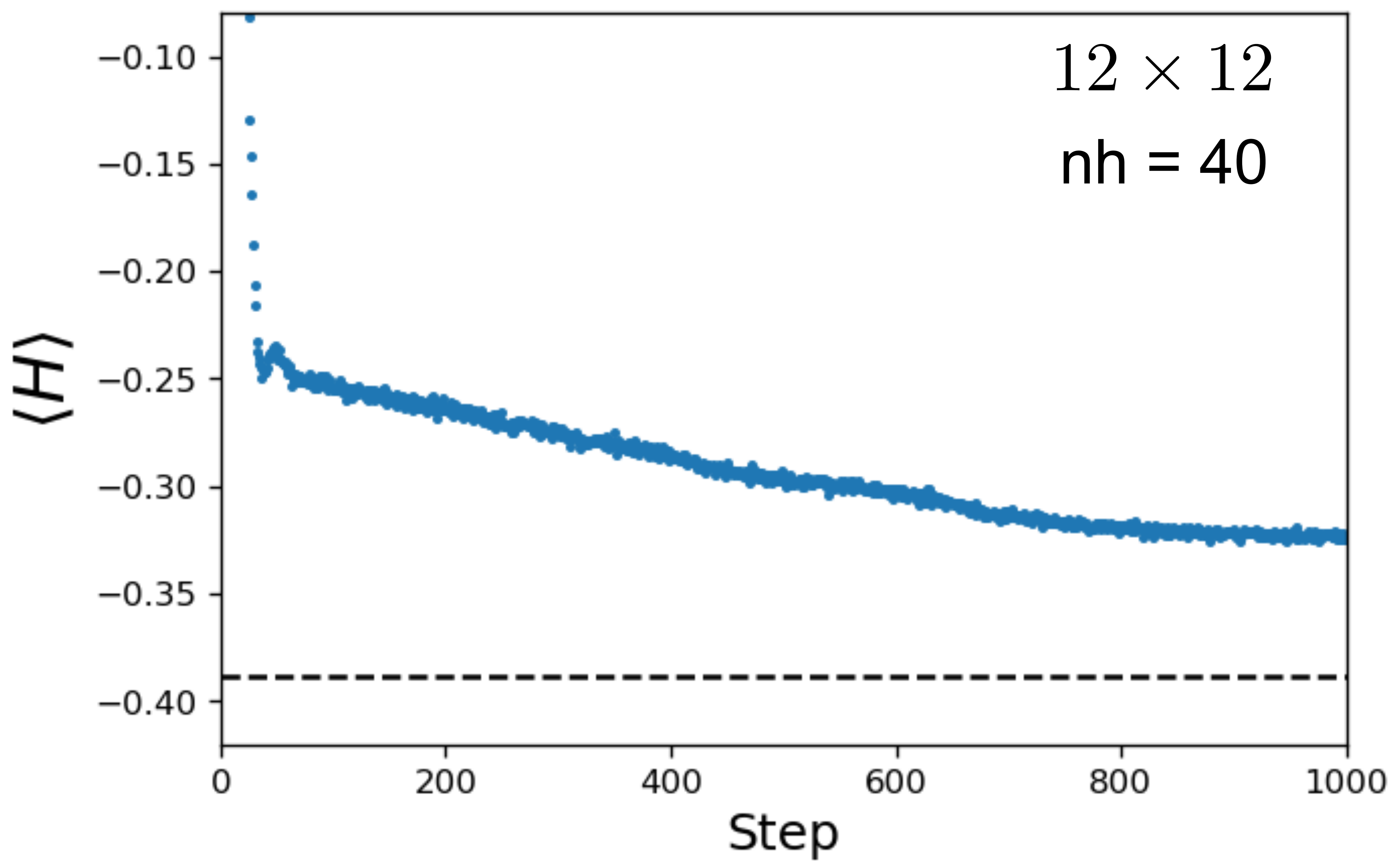


$$S_{\mathrm{topo}} = -S_{A_1} + S_{A_2} + S_{A_3} - S_{A_4}$$

What use is limited experimental data?

Neural network wavefunctions allow for model parameter optimization in two ways:





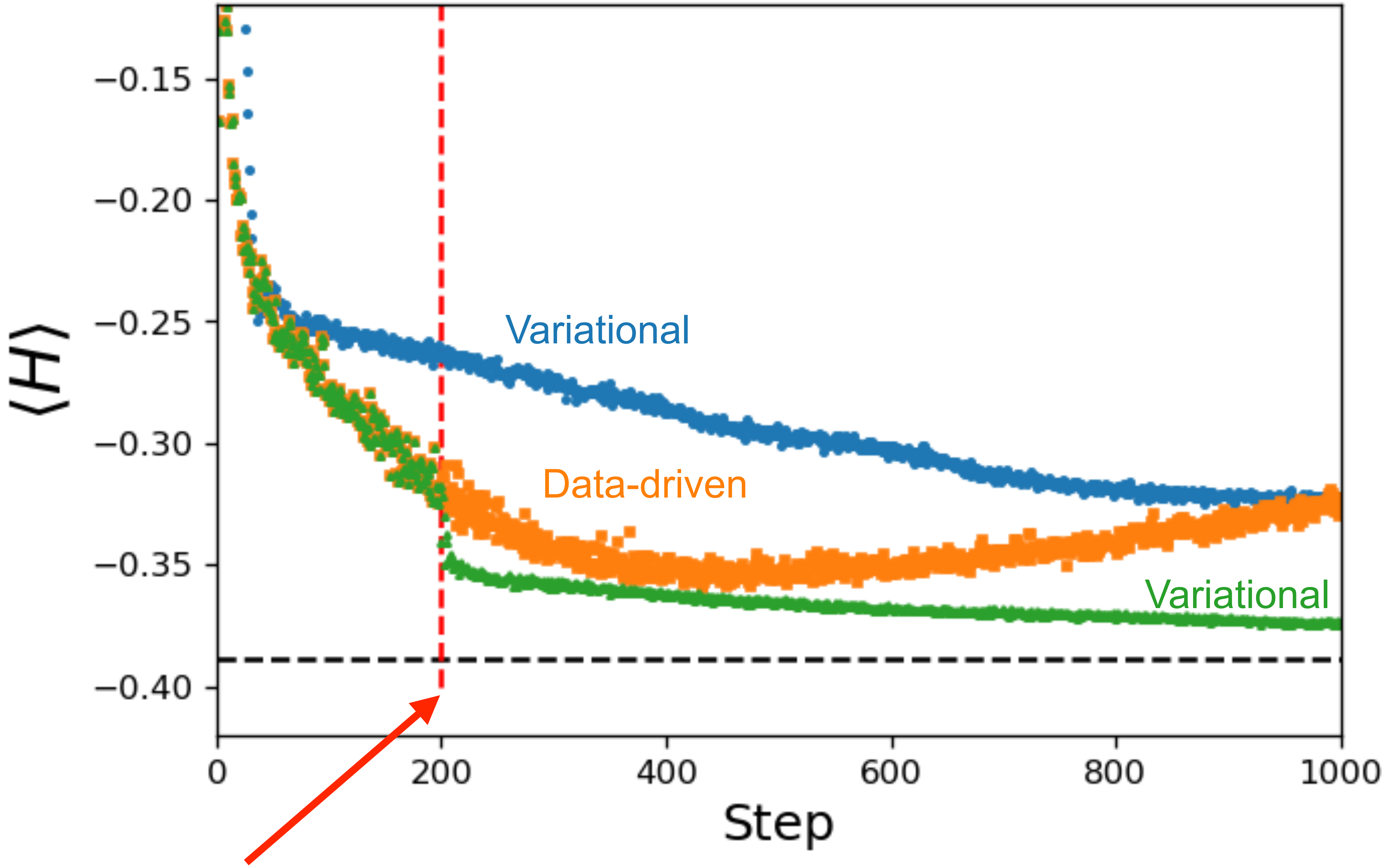
Data-driven, e.g. with the K-L divergence

Variationally (with knowledge of the Hamiltonian)

$$\mathrm{KL}(p||p_\lambda) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{p_\lambda(\mathbf{x})} \geq 0$$

$$\langle \psi_\lambda | H | \psi_\lambda \rangle$$

What use is limited experimental data?



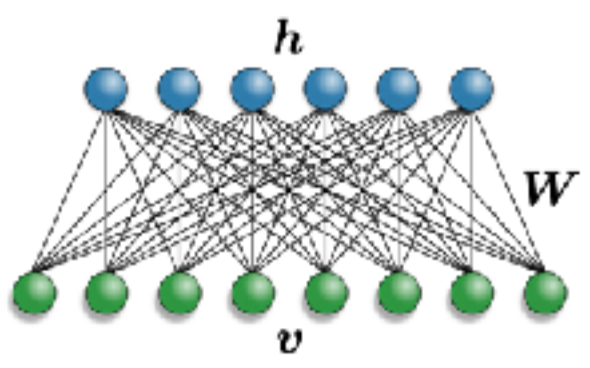
Keep parameters, switch cost functions

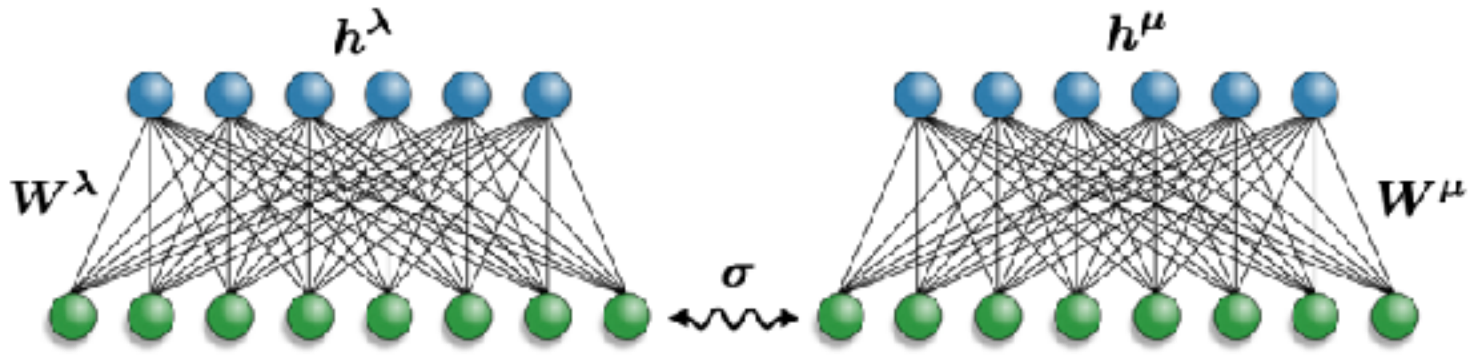
Complex quantum states

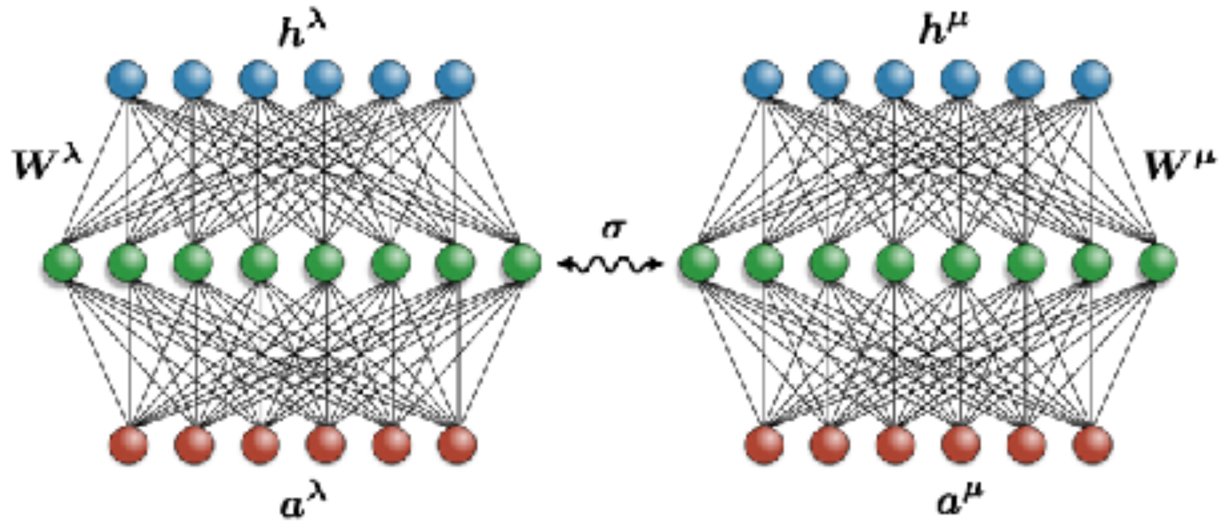
Torlai, Mazzola, Carrasquilla, Troyer, RGM, Carleo, Nature Physics 14, 447 (2018)
Torlai and RGM, Annual Review of Condensed Matter Physics 11:325-344 (2020)
RGM, Carleo, Carrasquilla, Cirac, Nature Physics 15, 887 (2019)

- Conventional generative models can be adapted to learn pure & mixed quantum states

sign free → pure wavefunction → density matrix







$\psi_\lambda(\mathbf{x}) \propto \sqrt{p_\lambda(\mathbf{x})}$

$\psi_{\lambda,\mu}(\mathbf{x}) \propto \sqrt{p_\lambda(\mathbf{x})}e^{i\phi_\mu(\mathbf{x})}$

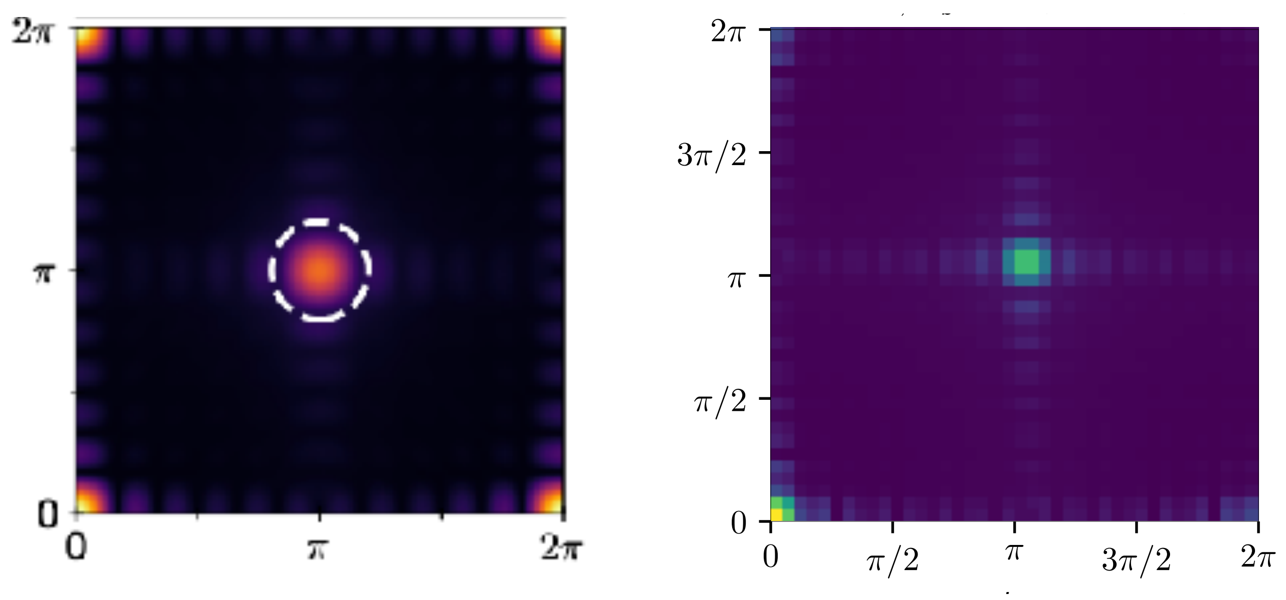
$\psi_{\lambda,\mu}(\mathbf{x},\mathbf{a}) \propto \sqrt{p_\lambda(\mathbf{x},\mathbf{a})}e^{i\phi_\mu(\mathbf{x},\mathbf{a})}$

$$\rho_{\lambda,\mu}(\mathbf{x},\mathbf{x}') = \sum_{\mathbf{a}} \psi_{\lambda,\mu}(\mathbf{x},\mathbf{a})\psi^*_{\lambda,\mu}(\mathbf{x}',\mathbf{a})$$

- Will make the data driven problem that much harder

$$\mathcal{L} = \sum_b^{N_b} \sum_{\mathbf{x}_b} \log |\psi_{\lambda,\mu}(\mathbf{x}_b)|^2$$

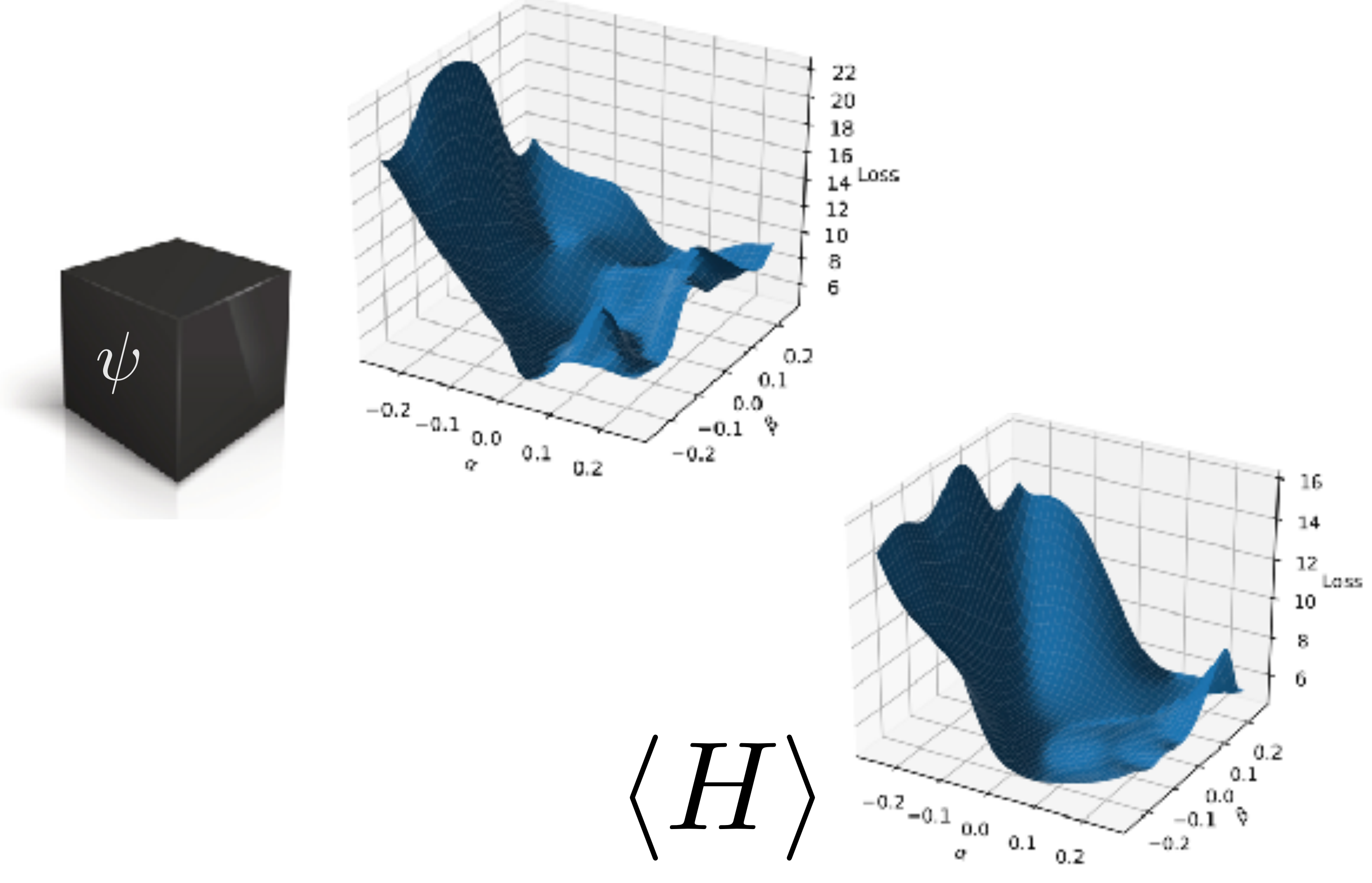
Discussion: Rydberg atom arrays



- A platform for exciting physics

- Classical simulations can reproduce current experiments - but for how long?

- Projective (experimental) measurement data opens up the possibility of combining *data-driven* with *variational* parameter learning.



- Experiments are capable of producing other Hamiltonians, including non-stoquastic models (eg. XXZ)

$$H = \sum_{i \neq j} J_{ij} \sigma_i^z \sigma_j^z + J'_{ij} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$$

Scholl *et al.*, arXiv:2107.14459