Title: Integrating Neural Networks with a Quantum Simulator for State Reconstruction

Speakers: Evert van Nieuwenburg

Collection: Machine Learning for Quantum Design

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Abstract: In this talk I will discuss how (unsupervised) machine learning methods can be useful for quantum experiments. Specifically, we will consider the use of a generative model to perform quantum many-body (pure) state reconstruction directly from experimental data. The power of this machine learning approach enables us to trade few experimentally complex measurements for many simpler ones, allowing for the extraction of sophisticated observables such as the RÃ©nyi mutual information. These results open the door to integration of machine learning architectures with intermediate-scale quantum hardware.

Integrating Neural Networks and Quantum Simulators

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Quantum TiqTaqToe
Out now on Android & iOS!

The Team

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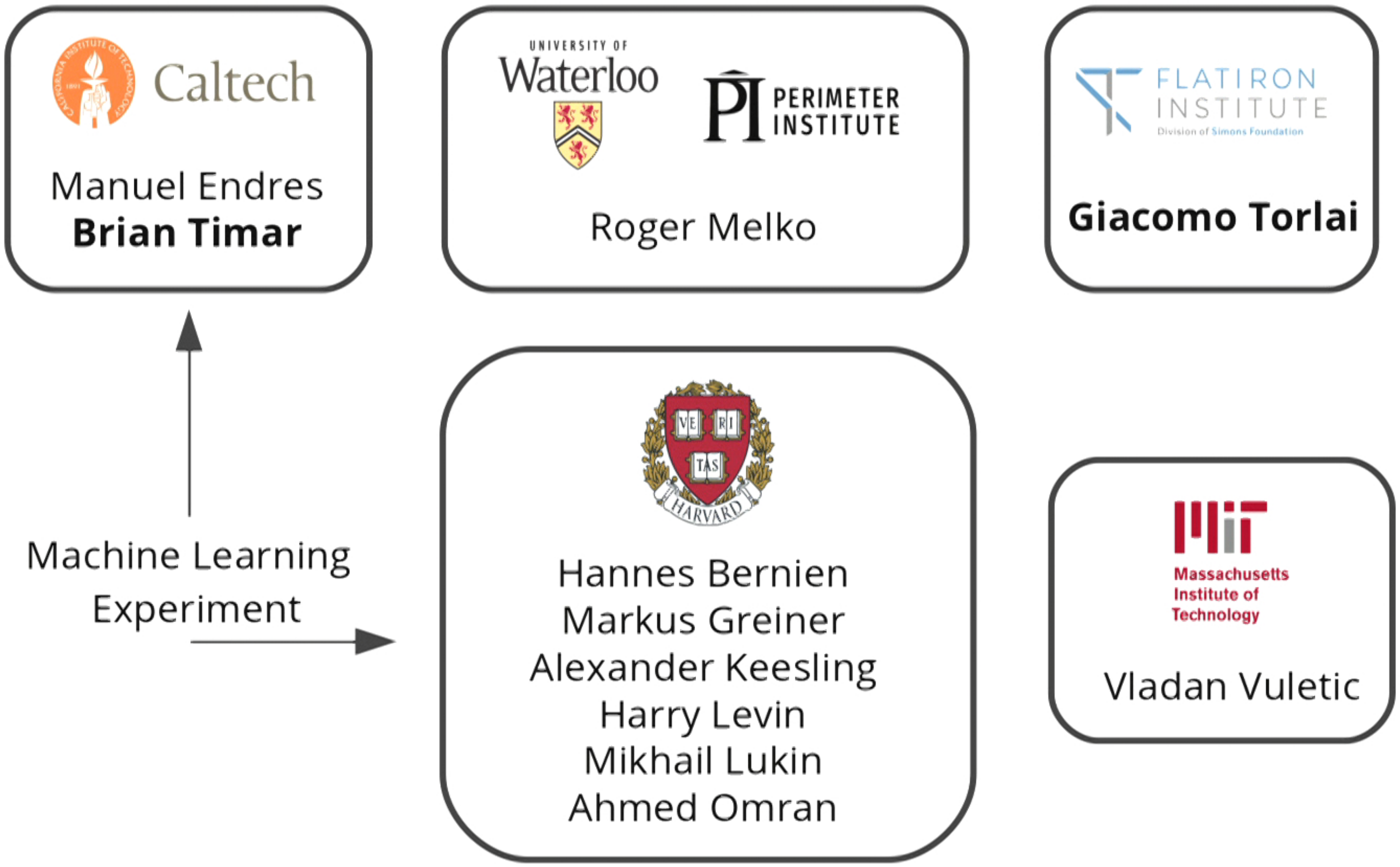
The Team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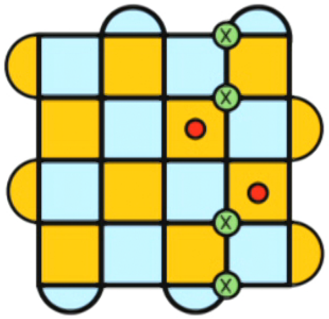
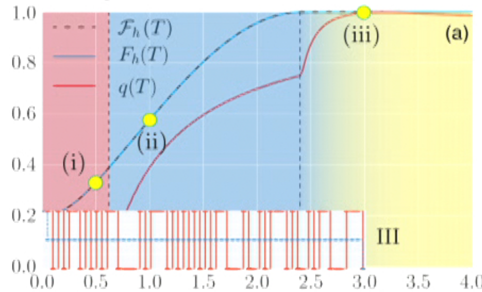
Context

Integrating machine learning & physics experiments

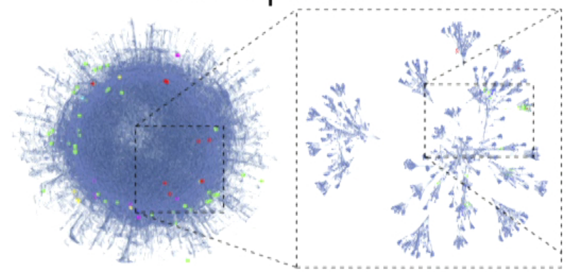
Quantum Error Correction



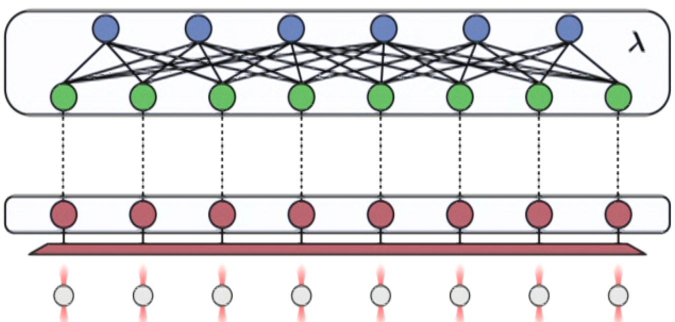
Quantum Control



Experimental Design and Optimization



State Reconstruction



Phases & Transitions

$\lambda_{\text{critical}}$

The setup

$$\boxed{\textbf{Experiment}} \longrightarrow \langle \hat{O} \rangle$$

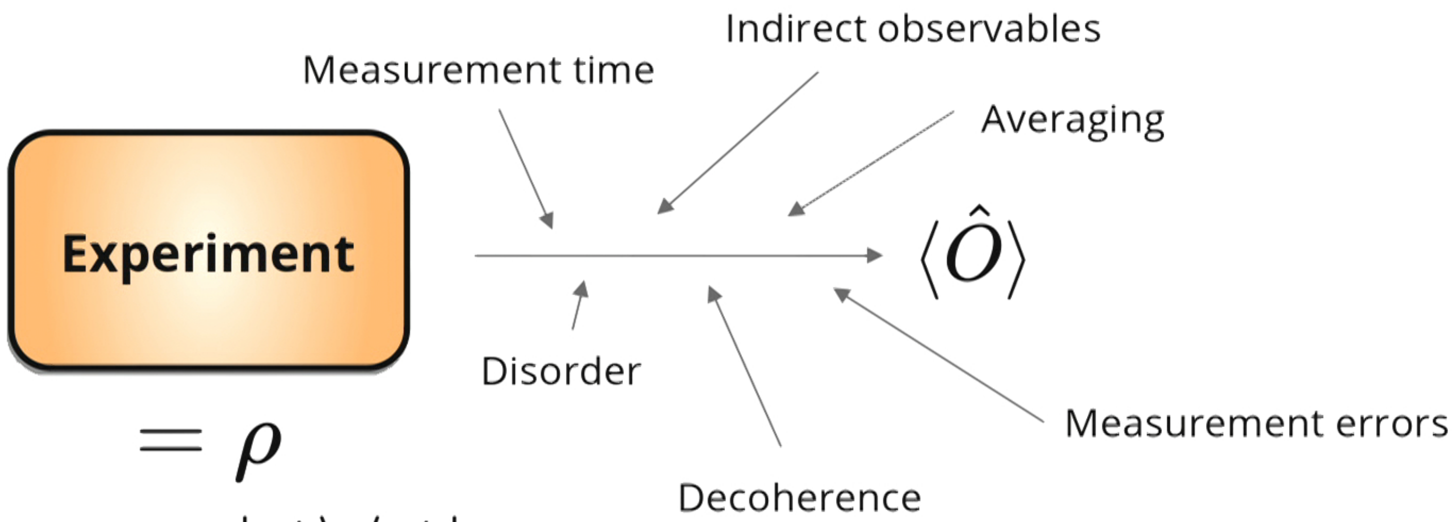
Averaging

$$= \rho$$

$$= |\psi\rangle\langle\psi|$$

$$= \mathrm{Tr}\left(\rho\, \hat{O}\right)$$

The setup



$$= \rho$$

$$= |\psi\rangle\langle\psi|$$

The setup

Experiment

$$= \rho$$

$$= |\psi\rangle\langle\psi|$$

$$\langle \hat{\sigma}_z \rangle_{\text{snapshots}}$$

Projective measurements!

“Raw” data!

The crux

Experiment

$$\langle \hat{\sigma}_z \rangle_{\text{snapshots}}$$

$= \rho$

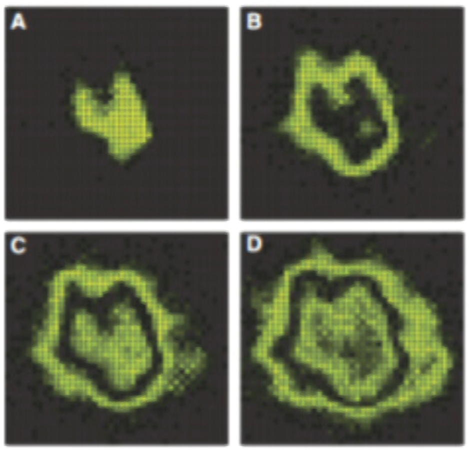
$= |\psi\rangle\langle\psi|$

Replace a complex measurement by many simpler ones!

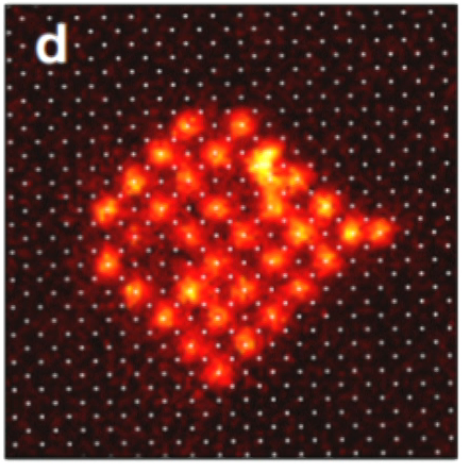
Projective measurements!

“Raw” data!

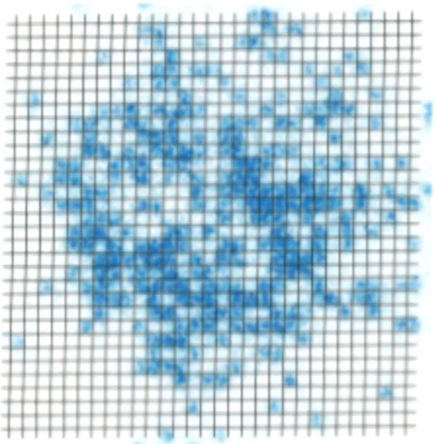
Snapshots are real



Bakr *et al* – Science (2010)

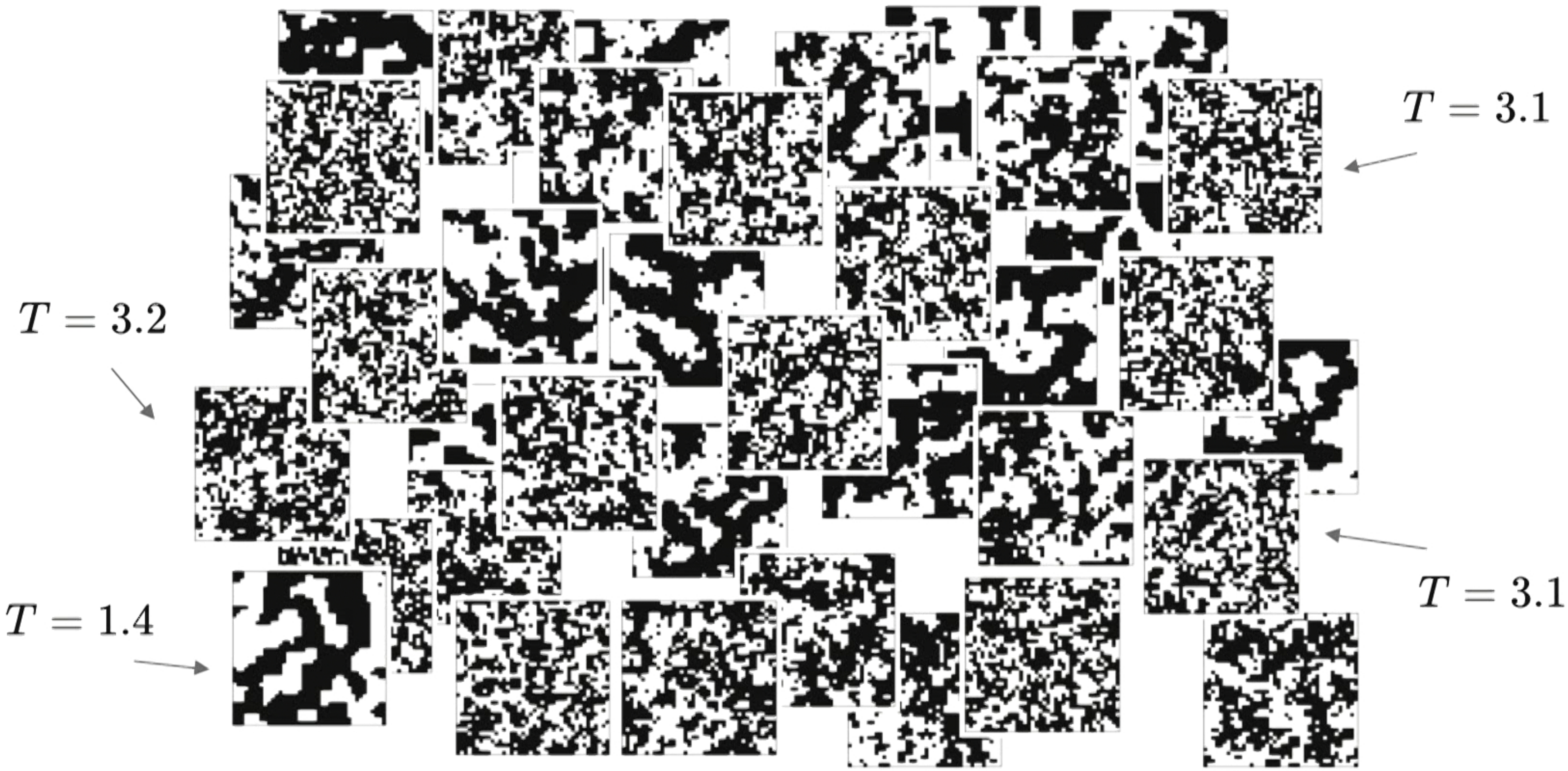


Weitenberg *et al* – Nature (2011)



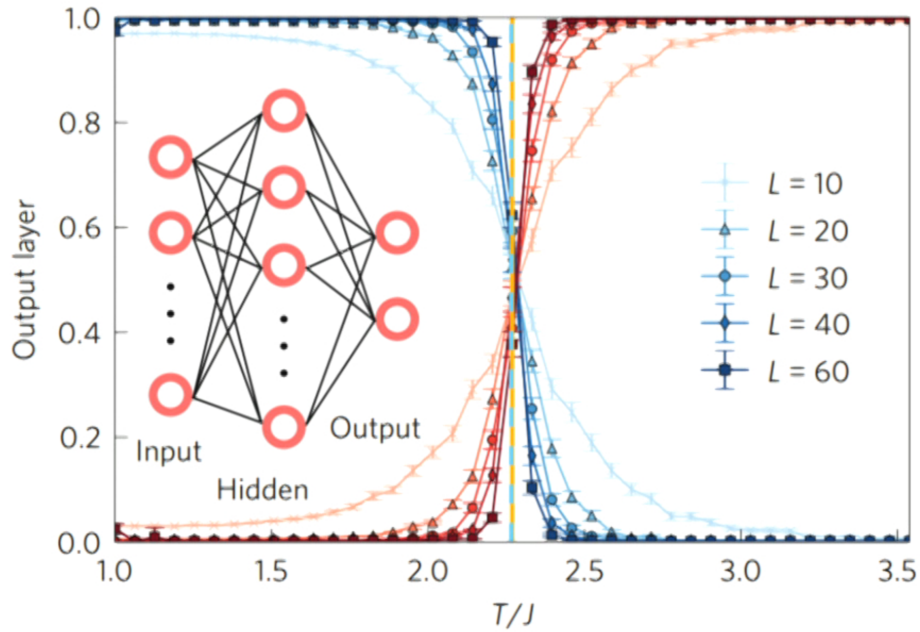
Greif *et al* – Science (2016)

Snapshots



Learning phases

Supervised learning!

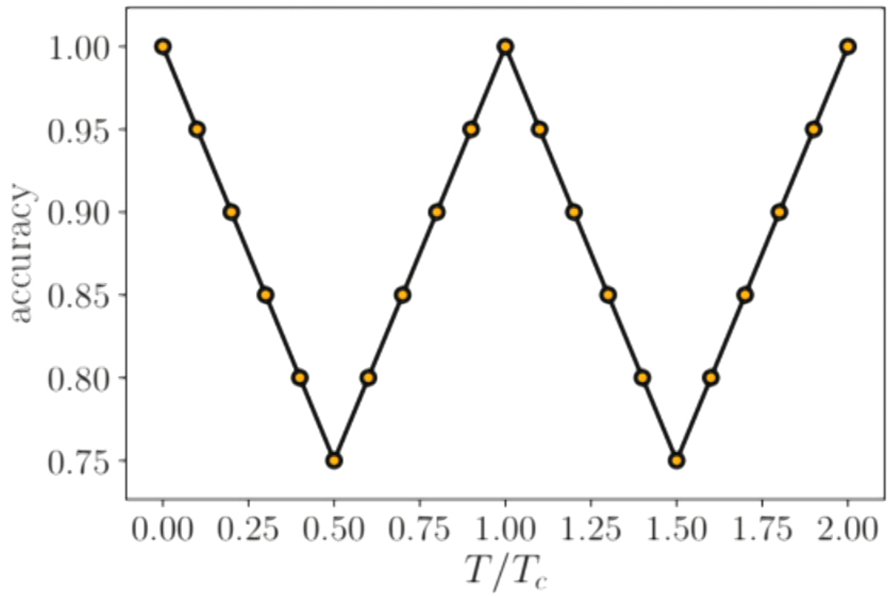


Carrasquilla and Melko – Nature Physics (2017)

Confused?

Semi-supervised learning!

Label = ?



Label = ?

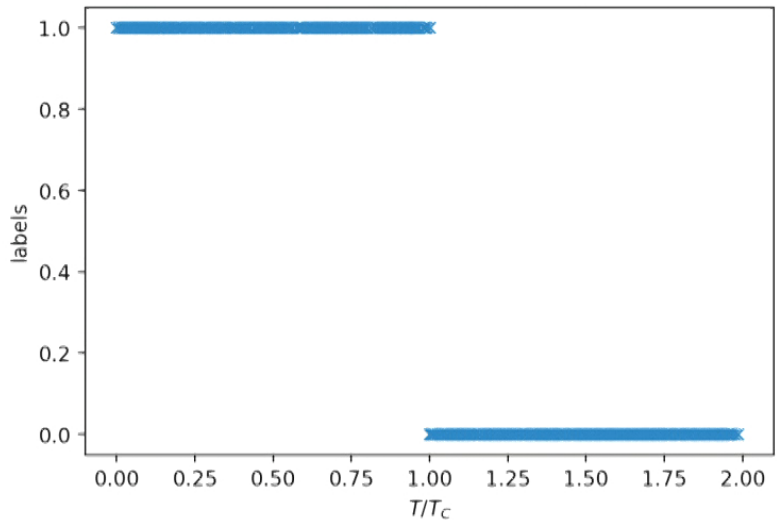
EvN, Y.-H. Liu and S. Huber – Nature Physics (2017)

Y.-H. Liu and EvN – PRL (2018)

Learning phases

Semi-supervised learning!

Label = ?



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Learning phases

Semi-supervised learning!

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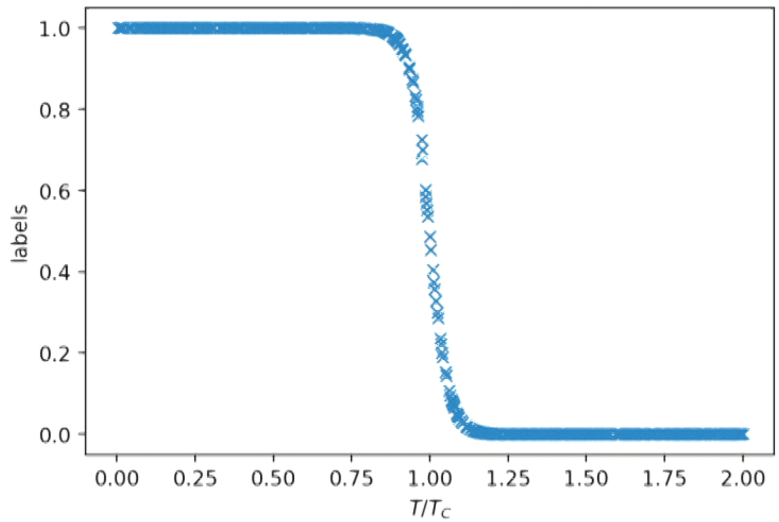

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Learning phases

Semi-supervised learning!

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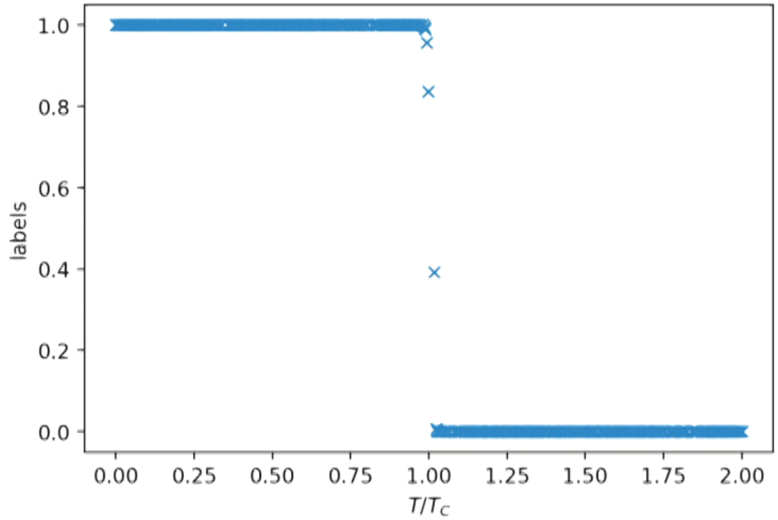

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Learning phases

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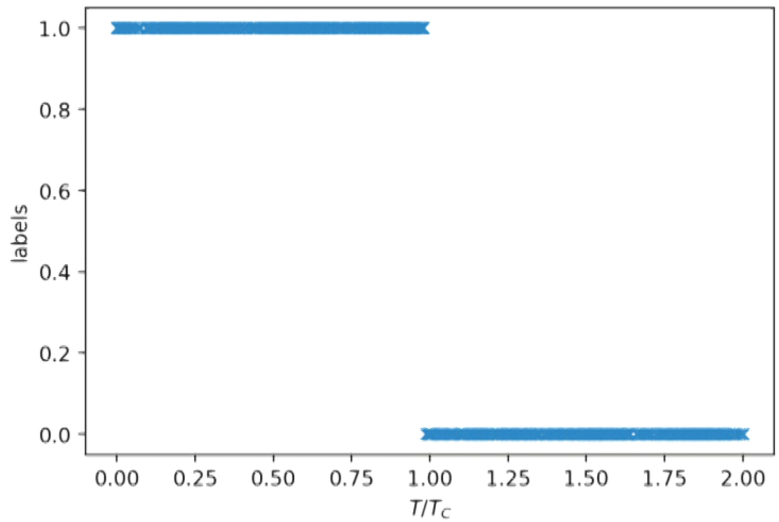

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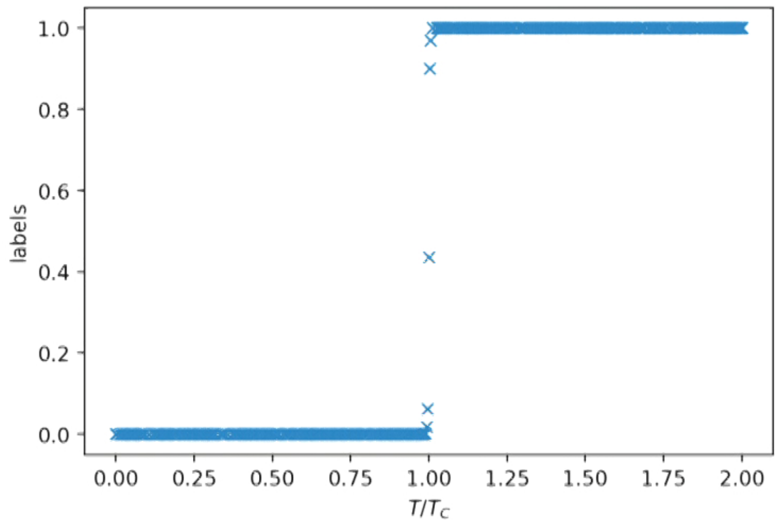
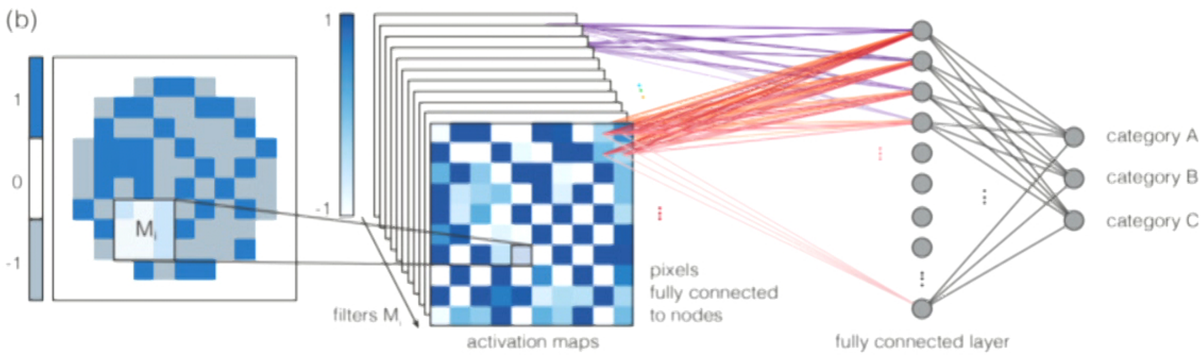


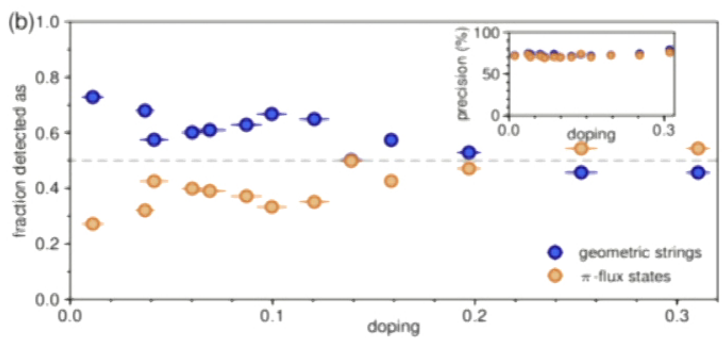
Label = ?

EvN, Y.-H. Liu and S. Huber – Nature Physics (2017)

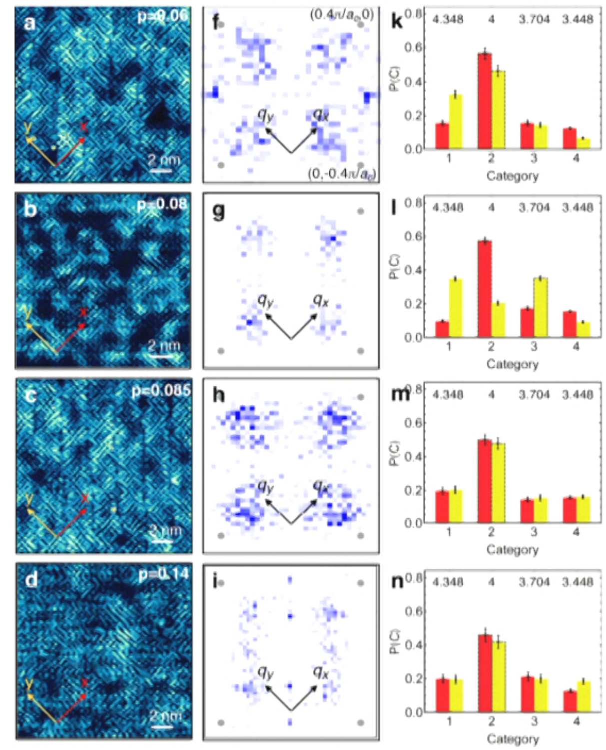
Y.-H. Liu and EvN – PRL (2018)

Experiments





A. Bohrdt *et al* – Nature Physics (2019)



Yi Zhang *et al* - Nature (2019)

Learning ~~phases~~ states

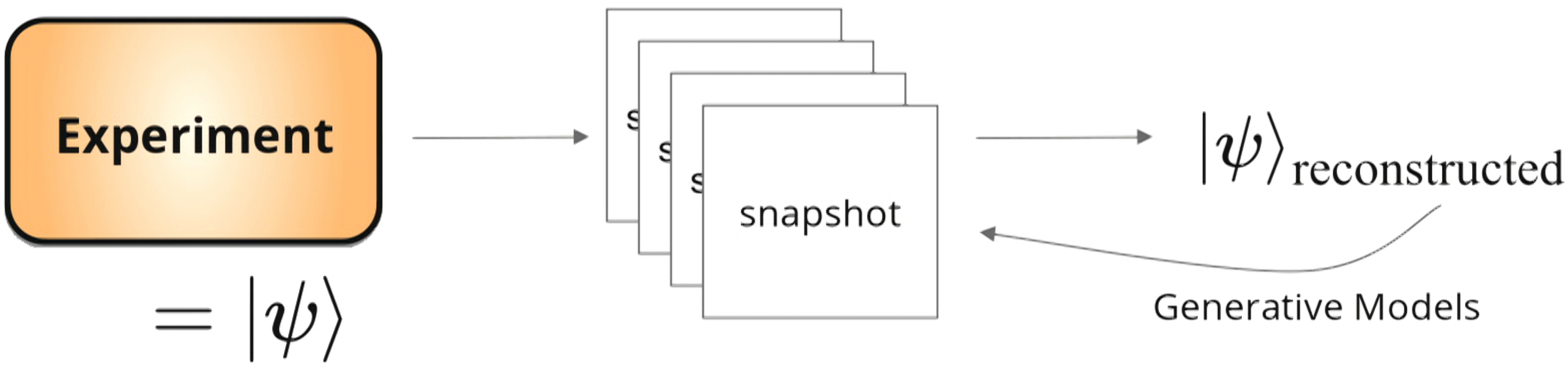
Experiment $\longrightarrow$ $\rho_{\text{reconstructed}}$

$|\psi\rangle_{\text{reconstructed}}$

$$= \rho$$

$$= |\psi\rangle\langle\psi|$$

Learning states



Example

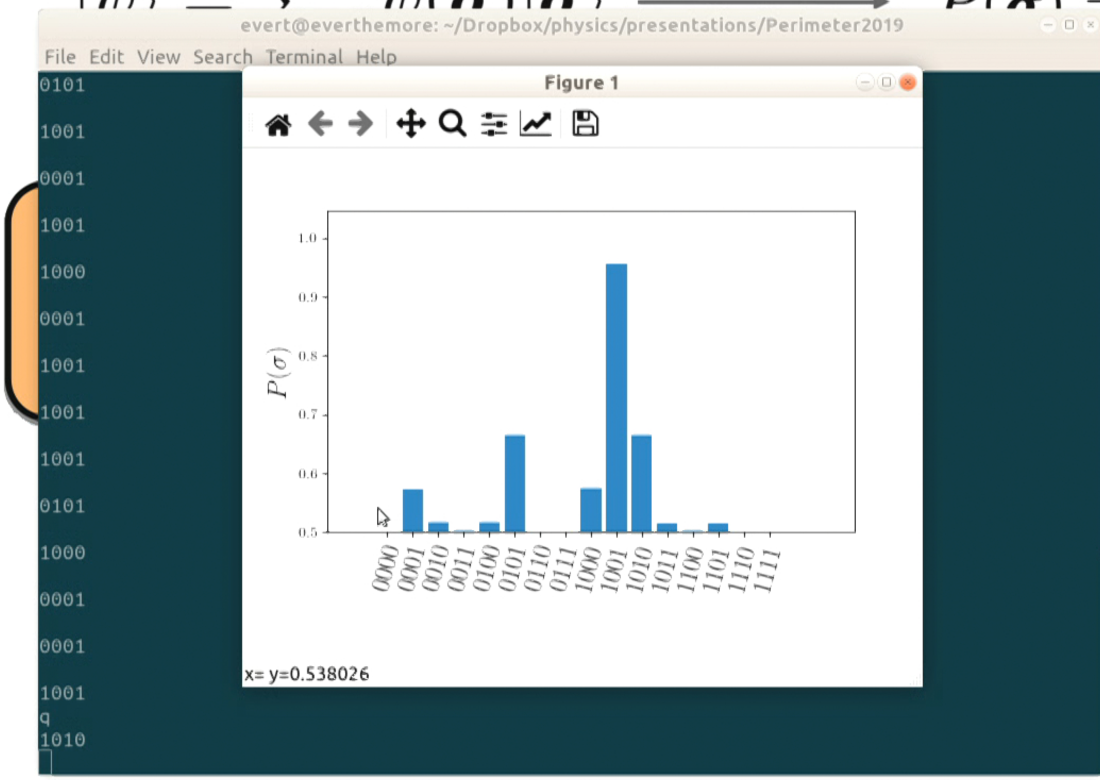
$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \psi(\boldsymbol{\sigma})|\boldsymbol{\sigma}\rangle \longrightarrow P(\boldsymbol{\sigma}) = |\psi(\boldsymbol{\sigma})|^2$$

$$\boxed{\textbf{Experiment}} \longrightarrow$$

$$= |\psi\rangle$$

Example

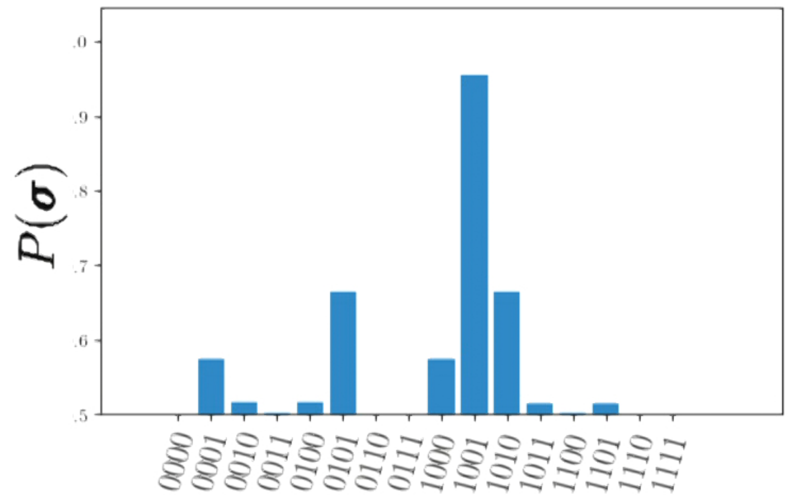
$$|\psi\rangle = \sum_{\sigma} \psi(\boldsymbol{\sigma})|\boldsymbol{\sigma}\rangle \longrightarrow P(\boldsymbol{\sigma}) = |\psi(\boldsymbol{\sigma})|^2$$



Example

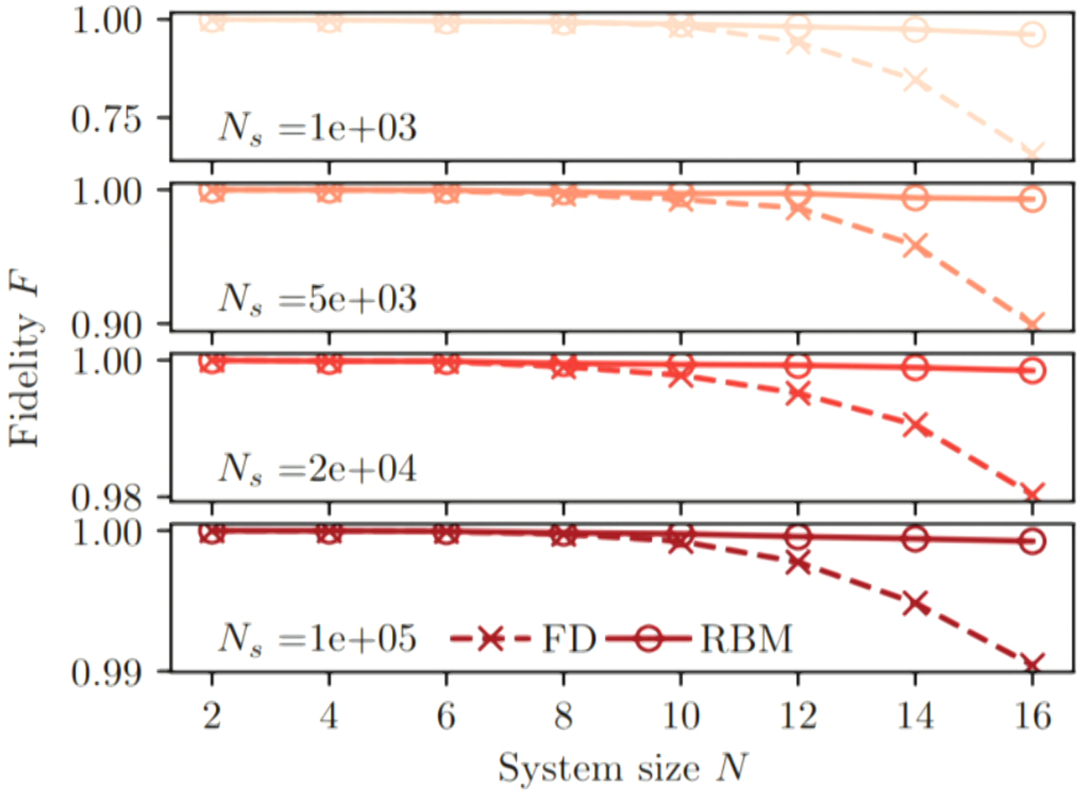
$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \psi(\boldsymbol{\sigma})|\boldsymbol{\sigma}\rangle \longrightarrow P(\boldsymbol{\sigma}) = |\psi(\boldsymbol{\sigma})|^2$$

$$= |\psi\rangle$$



$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \sqrt{P(\boldsymbol{\sigma})}|\boldsymbol{\sigma}\rangle$$

Why not use the histogram?



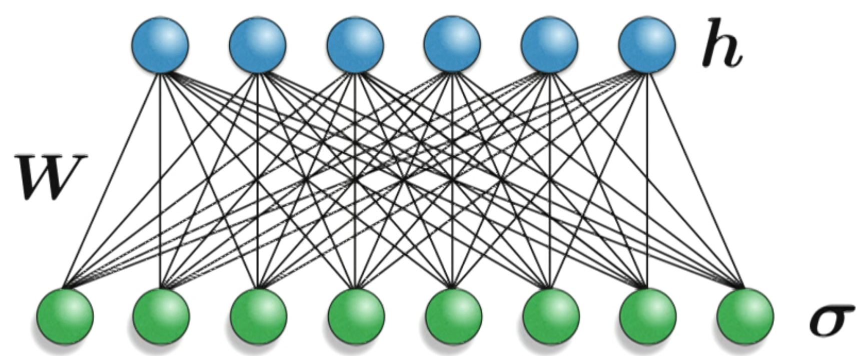
$$F_{\mathrm{FD}} \sim e^{-H_2}$$

A better representation

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \psi(\boldsymbol{\sigma})|\boldsymbol{\sigma}\rangle \longrightarrow P(\boldsymbol{\sigma}) = |\psi(\boldsymbol{\sigma})|^2$$

Exponentially many

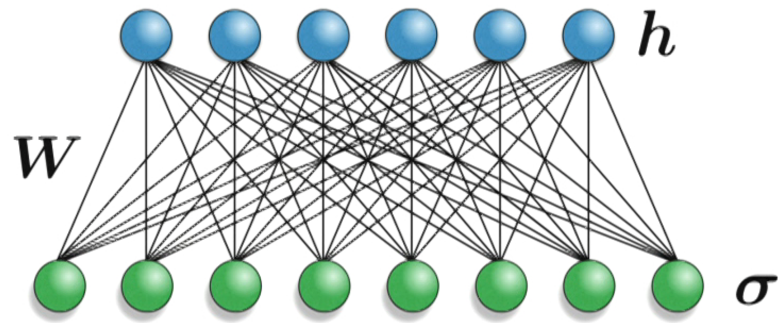
$P_W(\boldsymbol{\sigma}, \mathbf{h}) =$



$$P_W(\boldsymbol{\sigma}, \mathbf{h}) = \frac{1}{Z}\exp(-E_W(\boldsymbol{\sigma}, \mathbf{h}))$$

Restricted Boltzmann Machine

$$P_W(\boldsymbol{\sigma}, \mathbf{h}) =$$



$$P_W(\boldsymbol{\sigma}, \mathbf{h}) = \frac{1}{Z}\exp(\,-E_W(\boldsymbol{\sigma}, \mathbf{h})\,)$$

$$E_W(\boldsymbol{\sigma}, \mathbf{h}) = \boldsymbol{\sigma} \cdot W_{\sigma,h} \cdot \mathbf{h} + W_\sigma \cdot \boldsymbol{\sigma} + W_h \cdot \mathbf{h}$$

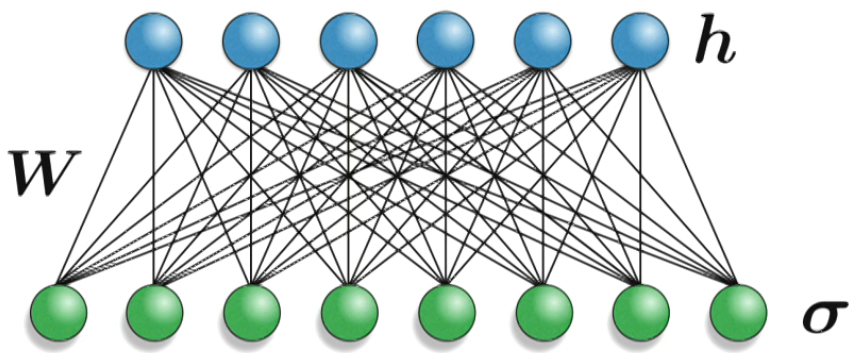
$$P_W(\boldsymbol{\sigma}) = \sum_{\mathbf{h}} P_W(\boldsymbol{\sigma}, \mathbf{h})$$

Method Summary

Experiment $\rightarrow$ 0 0 0 1 0 1 0 1
0 0 1 1 0 1 1 0
...
1 0 0 1 1 1 0 1 $\rightarrow$ $P_{\text{exp}}(\boldsymbol{\sigma})$

$= |\psi\rangle$

Tweak W to get identical!



$$P_W(\boldsymbol{\sigma}) = \sum_{\mathbf{h}} P_W(\boldsymbol{\sigma}, \mathbf{h})$$

$$|\psi\rangle_{\text{reconstructed}} = \sum_{\boldsymbol{\sigma}} \sqrt{P_W(\boldsymbol{\sigma})}|\boldsymbol{\sigma}\rangle$$

Training

Kullback Leibler Divergence

$$\mathrm{KL}(P_{\mathrm{exp}}||P_W) = \sum_{\boldsymbol{\sigma}} P_{\mathrm{exp}}(\boldsymbol{\sigma}) \log \frac{P_{\mathrm{exp}}(\boldsymbol{\sigma})}{P_W(\boldsymbol{\sigma})}$$

$$\simeq -\sum_{\boldsymbol{\sigma} \in \mathrm{exp}} \log P_W(\boldsymbol{\sigma})$$

Log-Likelihood

$$W \to W - \eta \nabla_W \, \mathrm{KL}(P_{\mathrm{exp}}||P_W)$$

Contrastive Divergence
Block Gibbs sampling

NetKet

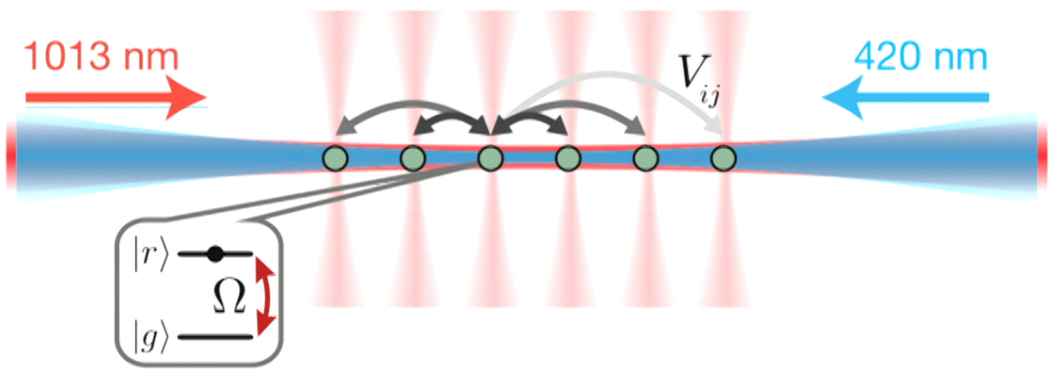
www.netket.org

QuCUMBER

github.com/PIQuIL/QuCumber

Quantum Simulator

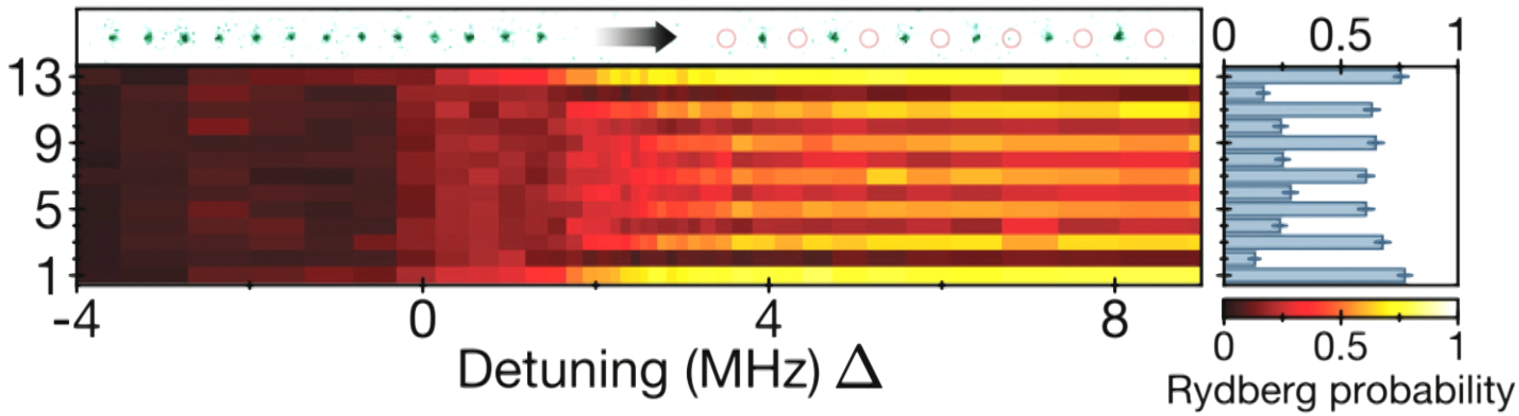
$$H = -\Delta \sum_i n_i - \frac{\Omega}{2} \sum_i \sigma_i^x + \sum_{i<j} \frac{V}{|i-j|^6} n_i n_j$$



Bernien *et al*, Nature (2017)

Quantum Simulator

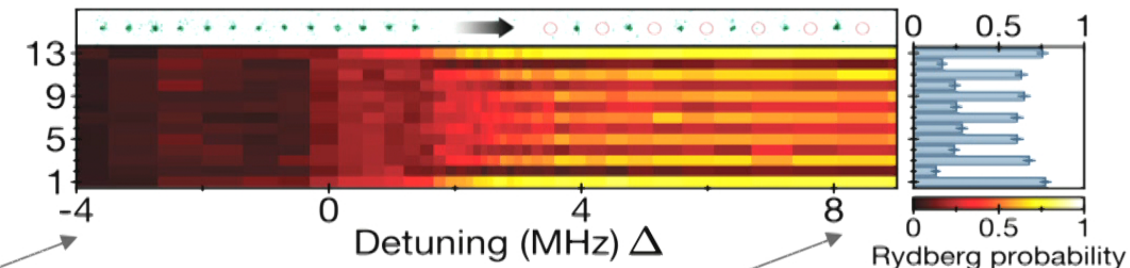
$$H = -\Delta \sum_i n_i - \frac{\Omega}{2} \sum_i \sigma_i^x + \sum_{i<j} \frac{V}{|i-j|^6} n_i n_j$$



Bernien *et al*, Nature (2017)

The Experiment

$$H = -\Delta \sum_i n_i - \frac{\Omega}{2} \sum_i \sigma_i^x + \sum_{i<j} \frac{V}{|i-j|^6} n_i n_j$$

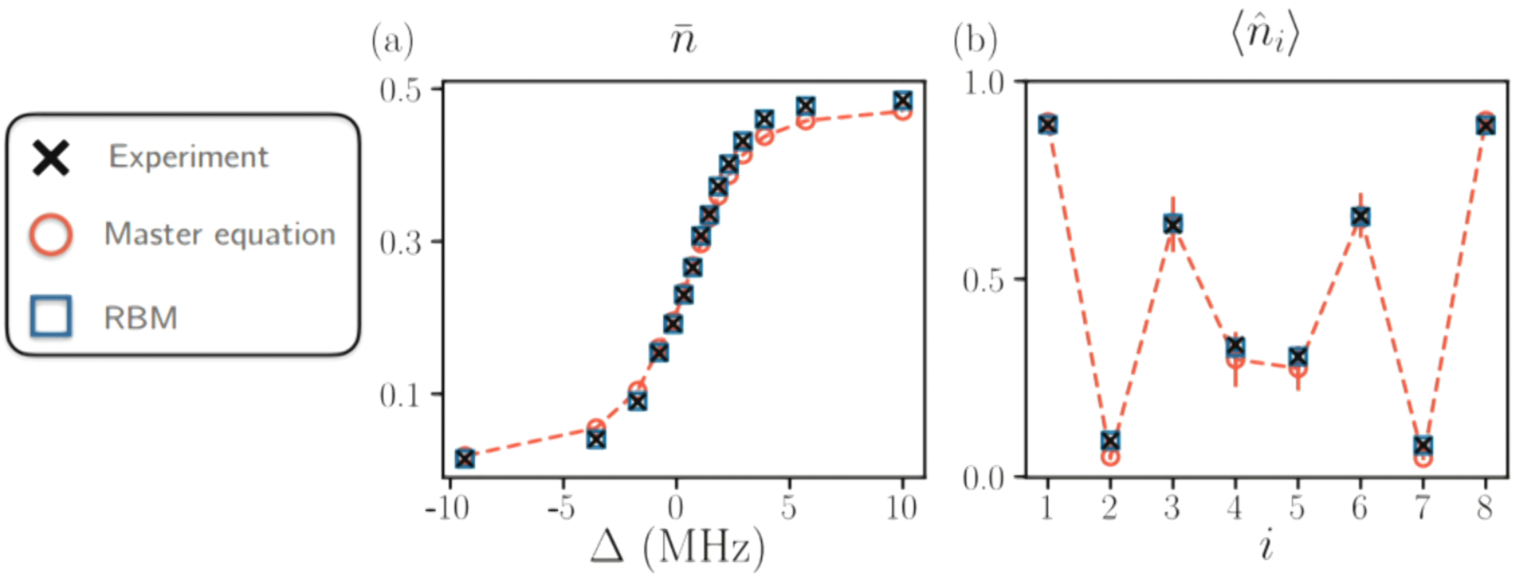


$|\psi(t=0)\rangle = |0\,0\,0\,0\,0\,0\,0\,0\rangle$

$|\psi(T)\rangle \approx \frac{1}{\sqrt{2}}|1\,0\,1\,0\,0\,1\,0\,1\rangle + \frac{1}{2}|1\,0\,1\,0\,1\,0\,0\,1\rangle + \frac{1}{2}|1\,0\,0\,1\,0\,1\,0\,1\rangle$

3000 snapshots at 15 different detunings
With decoherence and measurement errors!

The Experiment



Measurement errors

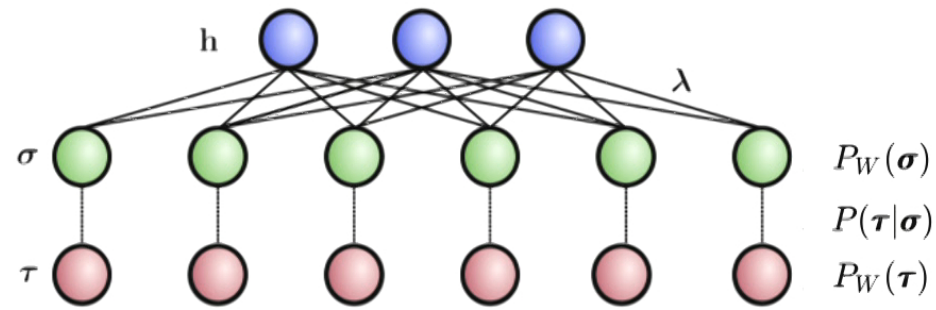
$$\text{Loss} = -\sum_{\boldsymbol{\sigma}\in\text{data}} \log P_W(\boldsymbol{\sigma})$$

$$\begin{array}{ccc} \boldsymbol{\sigma} & & \boldsymbol{\tau} \\ 0\,0\,0\,1\,0\,1\,0\,1 & & 0\,0\,0\,1\,0\,1\,0\,1 \\ 0\,0\,1\,1\,0\,1\,1\,0 & \xrightarrow{P(\boldsymbol{\tau}|\boldsymbol{\sigma})} & 0\,0\,1\,1\,0\,1\,1\,0 \\ \dots & & \dots \\ 1\,0\,0\,1\,1\,1\,0\,1 & & 1\,0\,0\,1\,1\,1\,0\,1 \end{array}$$

$$P_W(\boldsymbol{\tau}) = \sum_{\boldsymbol{\sigma}} P(\boldsymbol{\tau}|\boldsymbol{\sigma})\, P_W(\boldsymbol{\sigma})$$

$$\text{Loss} = -\sum_{\boldsymbol{\tau}\in\text{data}} \log P_W(\boldsymbol{\tau})$$

c.f. Torlai & Melko, PRL (2017)

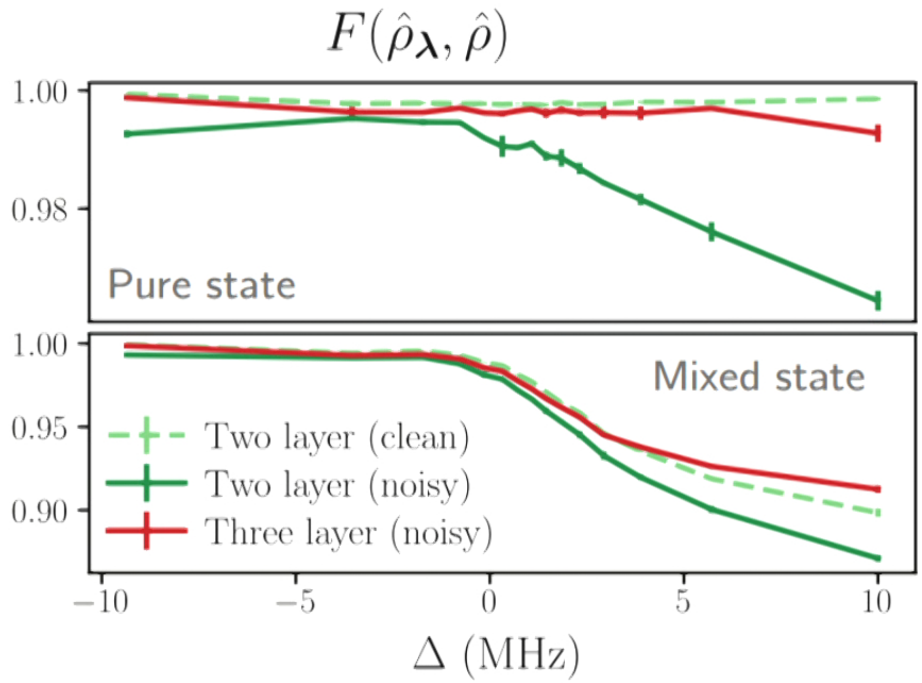


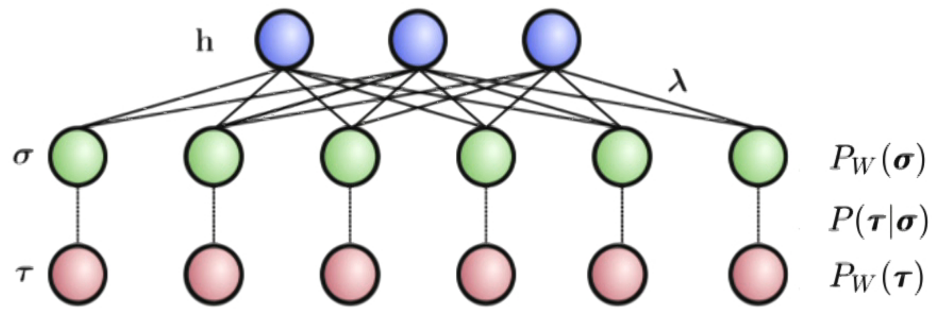
From the experiment:

$$P(0|1) = 0.04$$

$$P(1|0) = 0.01$$

Measurement errors

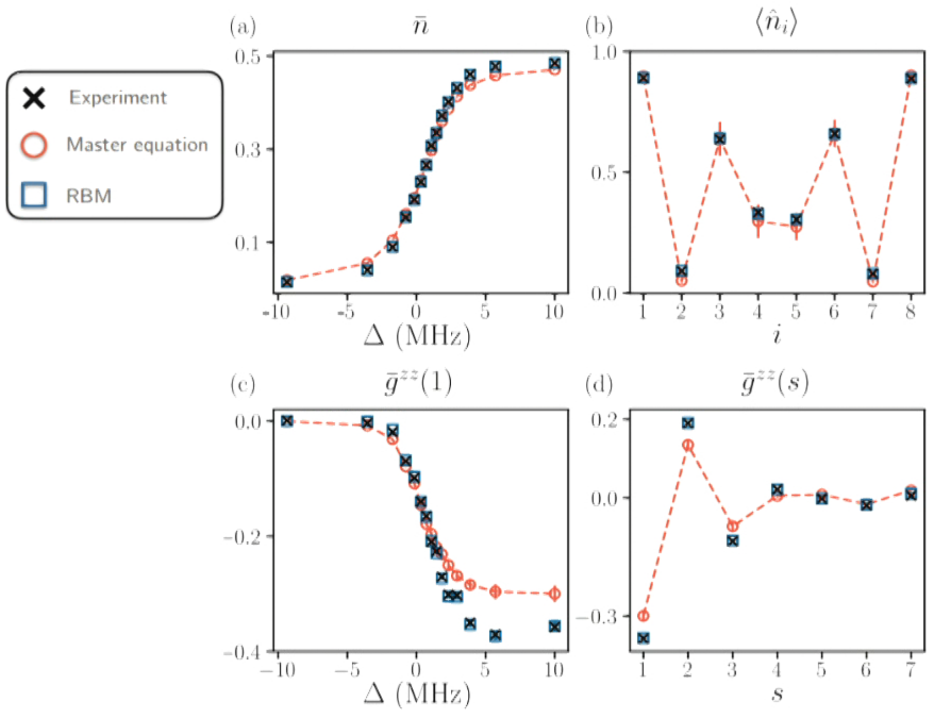


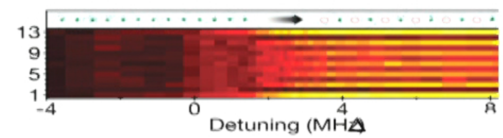


From the experiment:

$$P(0|1) = 0.04$$
$$P(1|0) = 0.01$$

Diagonal Observables

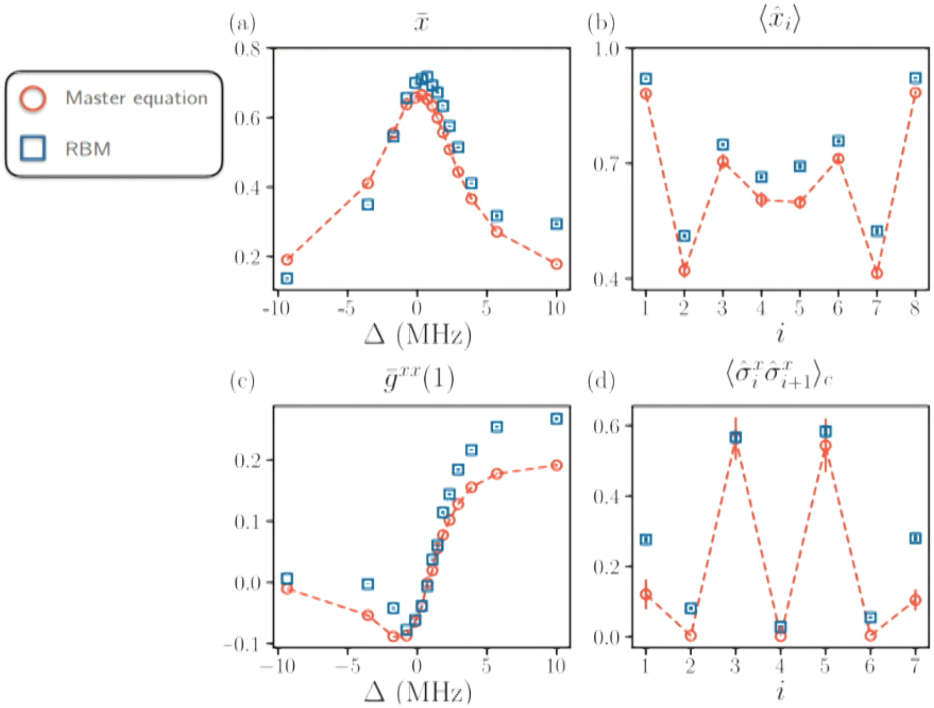


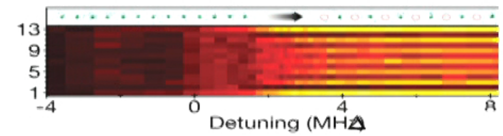


$$\bar{g}^{zz}(s) = \frac{1}{N-s} \sum_{i=1}^{N-s} \langle \sigma_i^z \sigma_{i+s}^z \rangle_c$$

$$|\psi(T)\rangle \approx \frac{1}{\sqrt{2}}|10100101\rangle + \frac{1}{2}|10101001\rangle + \frac{1}{2}|10010101\rangle$$

Off-Diagonal Observables





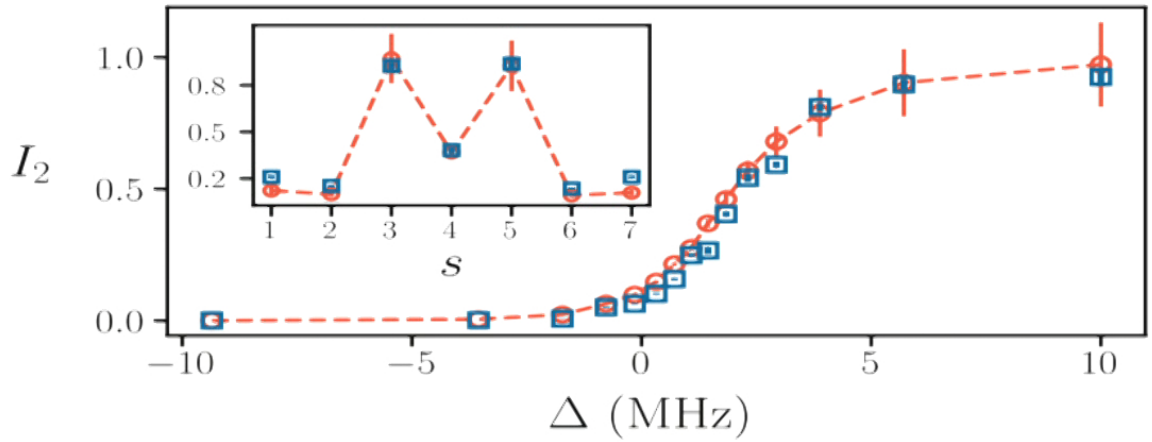
$$\bar{g}^{xx}(s) = \frac{1}{N-s} \sum_{i=1}^{N-s} \langle \sigma_i^x \sigma_{i+s}^x \rangle_c$$

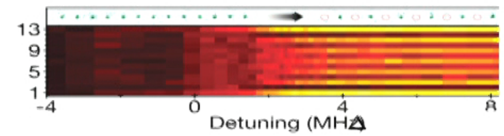
$$|\psi(T)\rangle \approx \frac{1}{\sqrt{2}}|10100101\rangle + \frac{1}{2}|10101001\rangle + \frac{1}{2}|10010101\rangle$$

Renyi Entropy

$$S_2(\rho) = -\log \mathrm{Tr}\, \rho^2$$

$$I_2(\rho) = S_2(\rho_A) + S_2(\rho_B) - S_2(\rho)$$

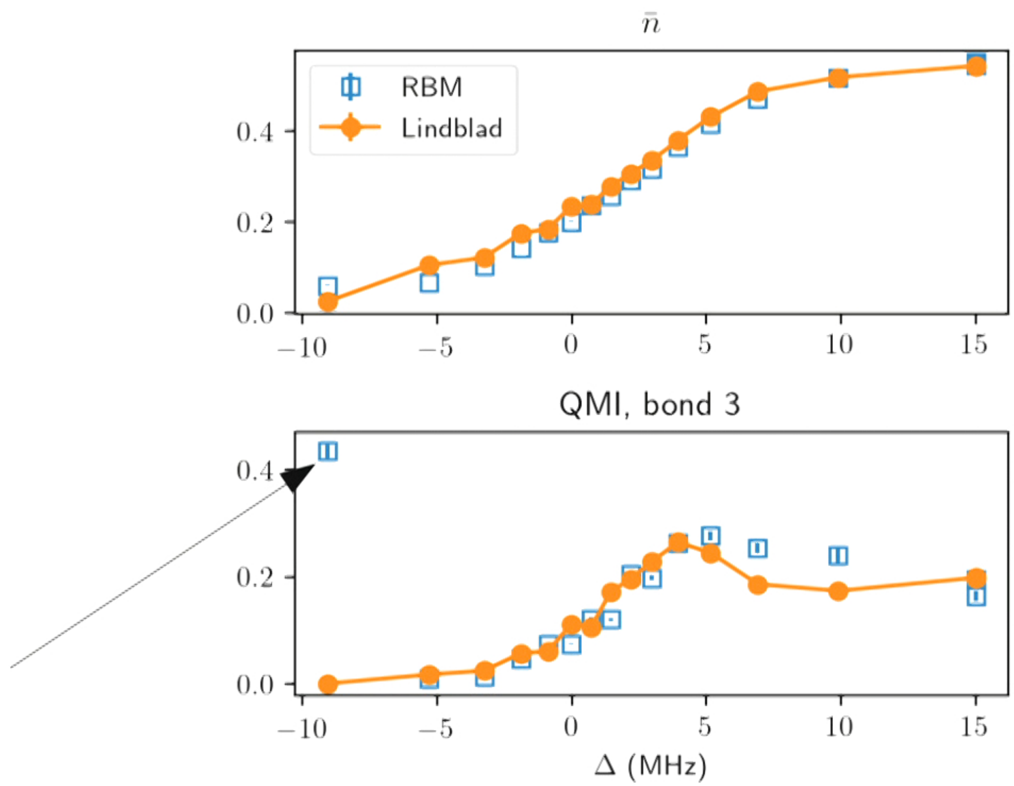




$$|\psi(T)\rangle \approx \frac{1}{\sqrt{2}}|10100101\rangle + \frac{1}{2}|10101001\rangle + \frac{1}{2}|10010101\rangle$$

Experimental debugging

9-atoms dataset



Summary

$$|\psi\rangle_{\text{reconstructed}} = \sum_{\boldsymbol{\sigma}} \sqrt{P_W(\boldsymbol{\sigma})}|\boldsymbol{\sigma}\rangle$$

Generative model
Restricted Boltzmann Machine

Trained on samples drawn from the **experiment**

Good empirical results for reconstructed properties, *despite*

- Non-pure
- Measurement errors

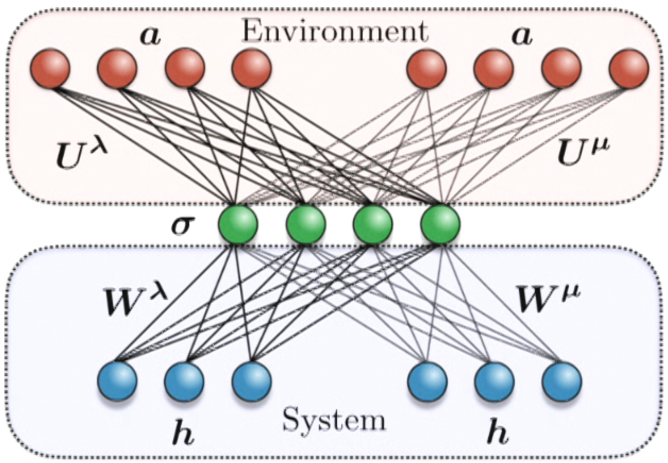
Extensions

1 Adding back in the sign-structure

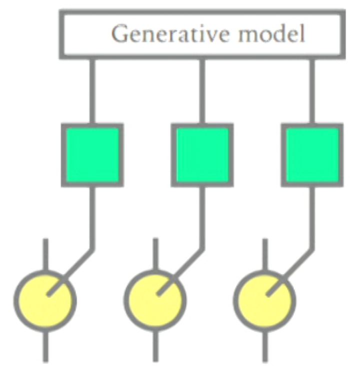
$$\psi_{W,W'} = \sqrt{P_W(\boldsymbol{\sigma})}\, e^{i\theta_{W'}(\boldsymbol{\sigma})}$$

Torlai *et al*, Nat. Phys (2018)

2 Mixed states



Torlai and Melko, PRL(2018)



Carrasquilla *et al*, Nat. Machine Intel (2019)