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Analyzing non equilibrium quantum states through snapshots with artificial networks

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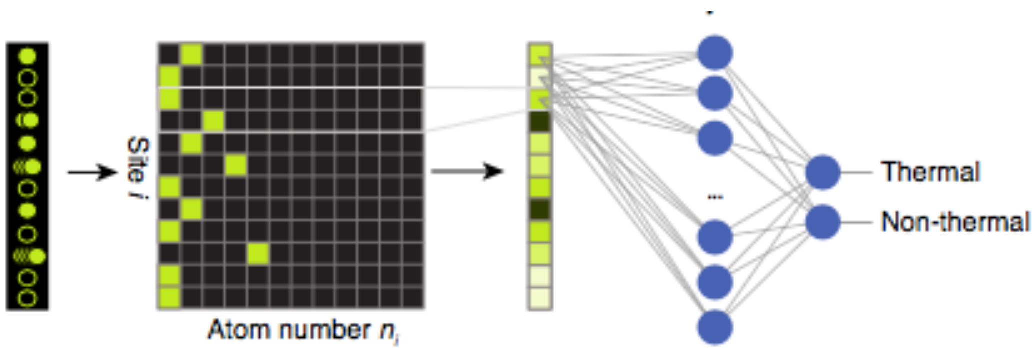
Introduction

- Analysis of non-equilibrium dynamics using neural networks and experimental data
- Network is trained with numerical data
- Experimental data is generated with quantum simulation devices

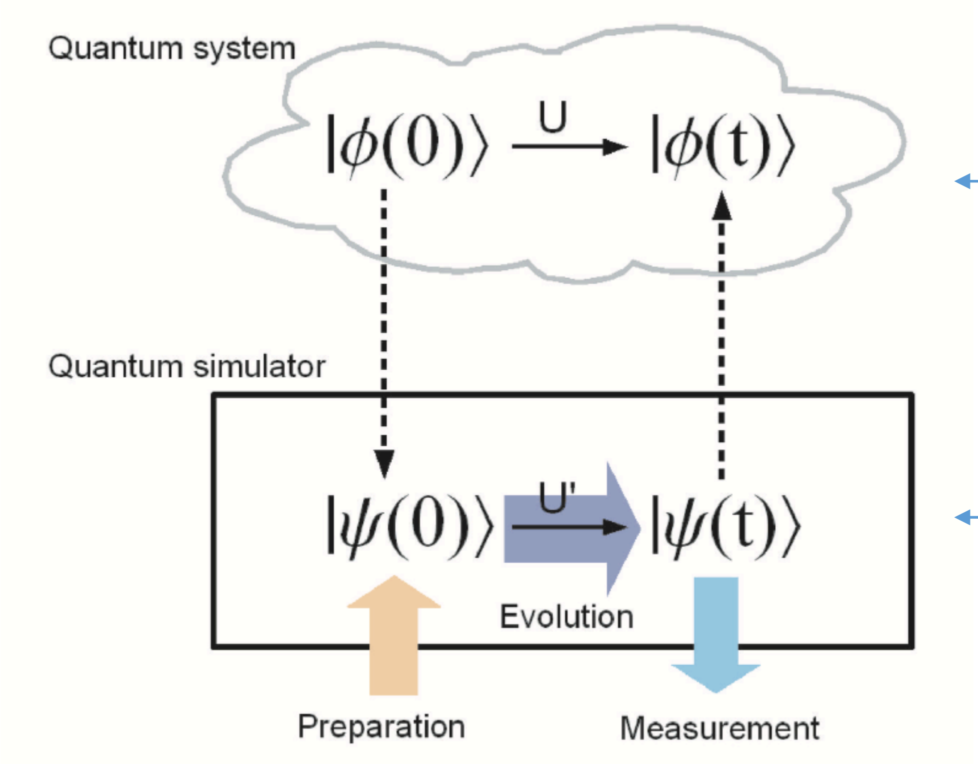


A. Bohrdt et al. arXiv:2012.11586v1, 2020

Quantum simulation

Quantum simulation
Basic idea

- Goal: access the time evolution of a quantum system



Quantum system of interest

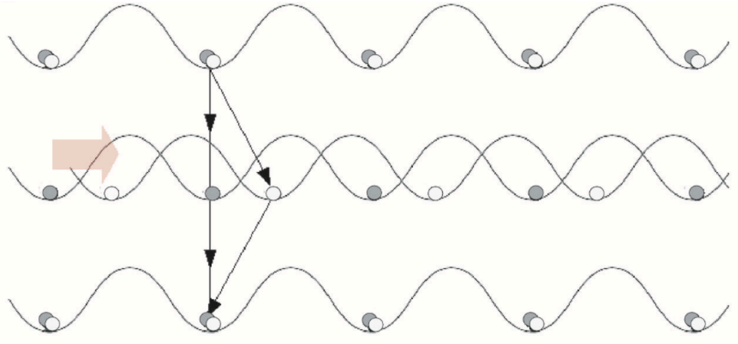
Artificial quantum system easy to manipulate

I. M. Georgescu, arXiv:1308.6253v3, 2014

Quantum simulation via ultra cold atoms Experimental realization

- Trap atoms into an optical potential consisting of two laser beams
- Manipulation of laser beams enables simulation of relevant Hamiltonian parameters

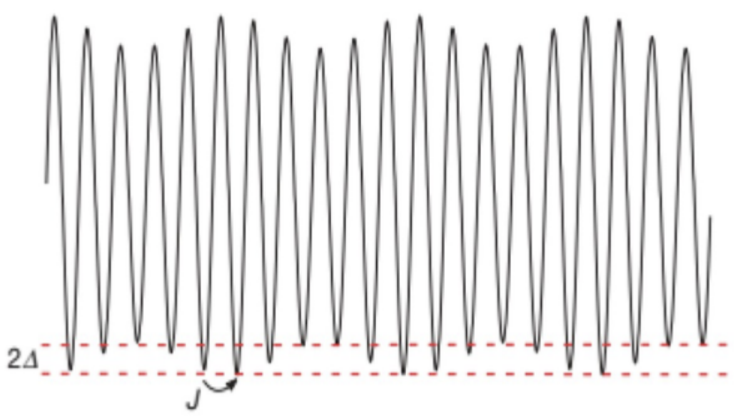
$$\hat{\mathcal{H}} = \sum_i \left[-J \left(\hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.} \right) + \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) + W h_i \hat{n}_i \right]$$



I. M. Georgescu, arXiv:1308.6253v3, 2014

Quantum simulation via ultra cold atoms Parameter manipulation

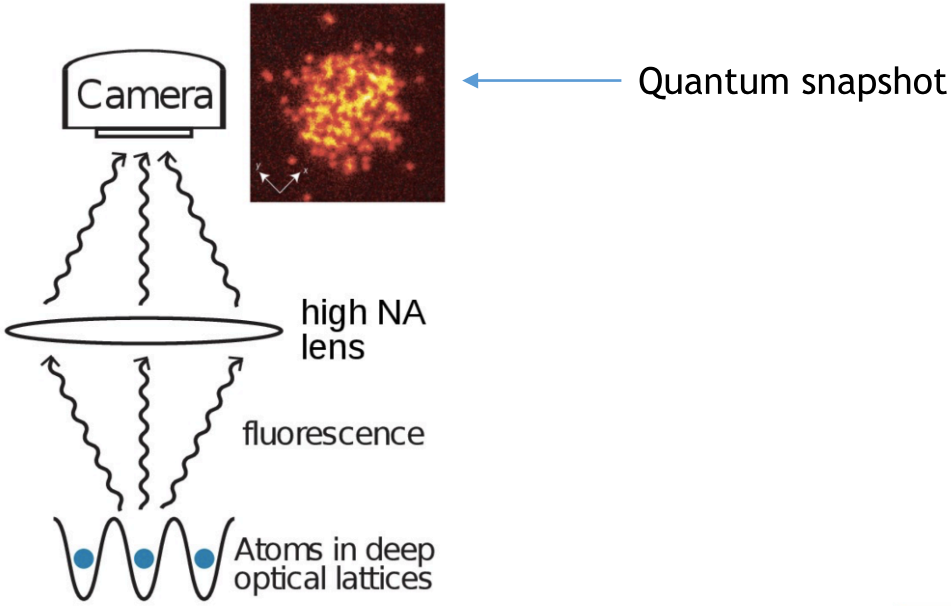
- Manipulation of disorder parameter is generated trough quasi periodic potentials
- Realized by superposition of two different laser beams



Florian Schäfer et al., nature review, 2020

Quantum simulation via ultra cold atoms
Generating snapshots

- Data acquisition using quantum gas microscope
- Allows to generate quantum snapshots



Florian Schäfer et al., nature review, 2020

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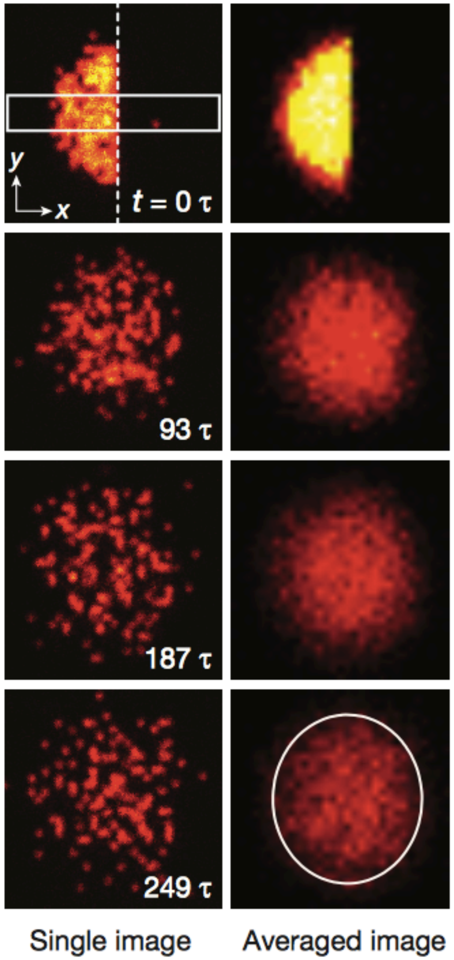
Many body localized phases

Many-body localized phases
Approaching thermal equilibrium

- Red dots represent position of atoms
- Quantum systems tend to thermal equilibrium on long time scales



Jae-yoon Choi et al., arXiv:1604.04178v1, 2016

Many-body localized phases
Approaching thermal equilibrium

- This behavior is suggested by the following calculation:

$$\langle O(t)\rangle = \langle\psi_0|e^{iHt}Oe^{-iHt}|\psi_0\rangle = \sum_{m,n}\langle\psi_0|m\rangle\langle m|O|n\rangle\langle n|\psi_0\rangle \cdot e^{-i(E_n-E_m)t}$$

oscillates fast for m unequal to n and if t >> 1

$\Rightarrow$ sum of these terms approaches zero

$$= \sum_n |\langle\psi_0|n\rangle|^2 \langle n|O|n\rangle$$

$\Rightarrow$ Which gives the diagonal elements of the observable depending on the initial state

$\Rightarrow$ Assume diagonal elements are effectively constant, then we approach the expectation value of the micro canonical ensemble

Josh M Deutsch Physical Review A 43.4 (1991)

Many-body localized phases
Eigenstate thermalization hypothesis

- For an observable on long time scales the diagonal matrix elements are a smooth function of the energy, matching its micro canonical expectation value

$$\langle n|O|n\rangle \simeq \bar{O}(E)$$

- Off-diagonal matrix elements will vanish in the thermodynamic limit exponentially fast

Josh M Deutsch Physical Review A 43.4 (1991)

Many-body localized phases
Avoiding thermalization with disorder

$$H_{\mathrm{rfH}} = \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z) - \sum_i h_i S_i^z$$

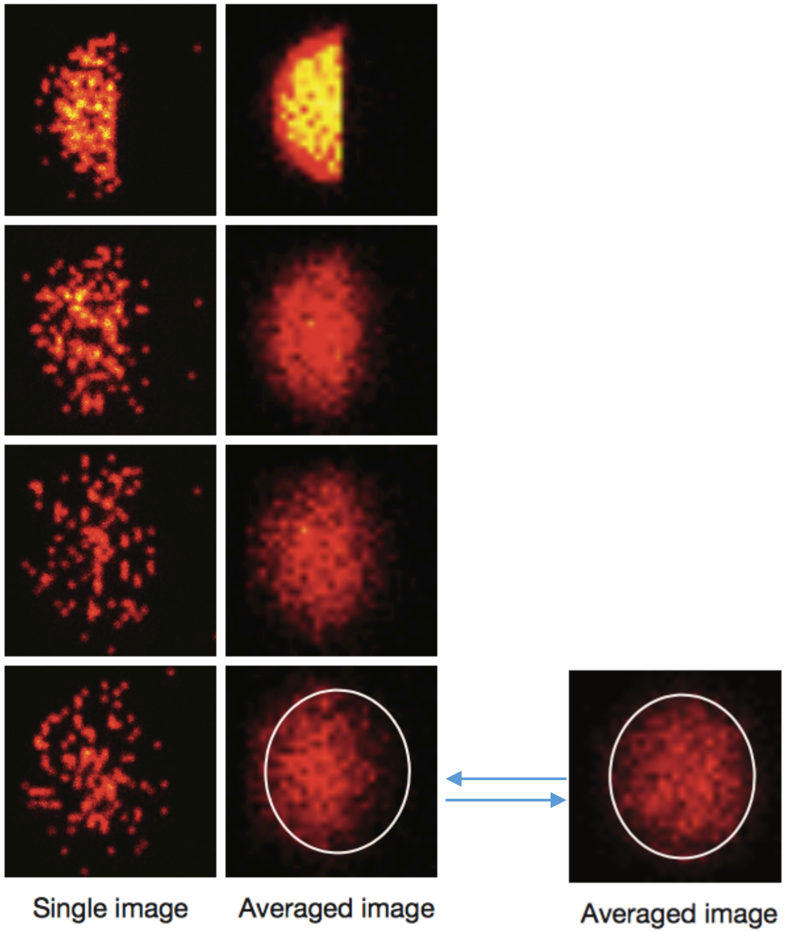
$$h \to \infty \qquad \longrightarrow \qquad |\uparrow\downarrow\downarrow\uparrow\ldots\rangle$$

Eigenstates become product states contradicting the ETH

Here the question arises at which finite value of h the phase transition actually occurs?

Many-body localized phases
Avoiding thermal equilibrium

- For higher disorder values and on long time scales the positions of the atoms are less evenly distributed



Jae-yoon Choi et al., arXiv:1604.04178v1, 2016

Analysis of non-equilibrium quantum states

Analysis of non-equilibrium quantum states
The model

- Consider 1D Bose-Hubbard model

Interaction

Disorder

$$\hat{\mathcal{H}} = \sum_i \left[-J \left(\hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.} \right) + \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) + W h_i \hat{n}_i \right]$$

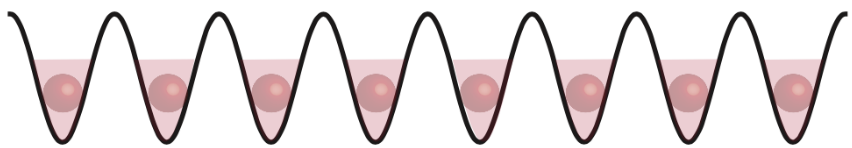
Hopping

Number operator

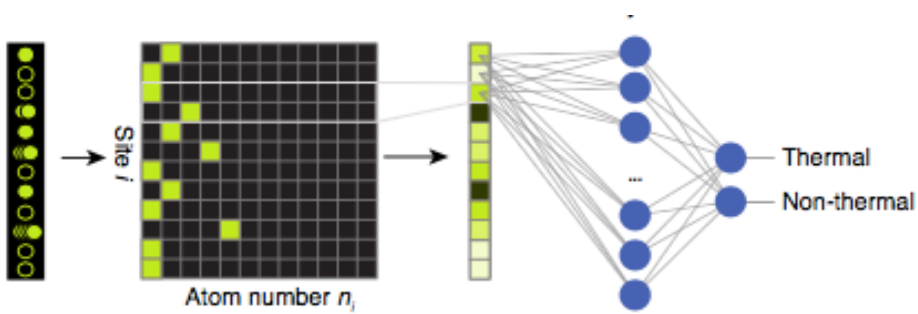
- Numerical snapshots are provided by exact diagonalization (where the atom number per site is the observable of interest)
- Experimental snapshots are provided by quantum simulation
- Snapshots represent time-evolution of the wave function

Analysis of non-equilibrium quantum states
Training the neural network

- Train network to distinguish snapshots of extremal cases of disorder strength after a global quench, starting with one atom per site



- The network is trained to label the input as equilibrium/ thermal or as MBL/non-thermal



A. Bohrdt et al. arXiv:2012.11586v1, 2020

Analysis of non-equilibrium quantum states
The cross entropy cost function

$$\mathcal{L}(X,Y) = -\frac{1}{n}\sum_{i=1}^{n} y^{(i)} \ln a(x^{(i)}) + \left(1 - y^{(i)}\right) \ln\left(1 - a(x^{(i)})\right)$$

labels for input examples

Output of network

set of input examples

- Suitable cost function for classification problem
- The gradient penalizes stronger for bigger errors

Analysis of non-equilibrium quantum states
Cross entropy example

- Consider a two classes problem where 0 and 1 are the only possible labels
- Assume network gives output a = 0.9 but the correct label should actually be 0

Computing gradients with respect to a

Squared error function

$$L_{SE} = (y-a)^2 \longrightarrow L_{SE} = 0.81 \longrightarrow \frac{\partial L_{SE}}{\partial a} = 1.8$$

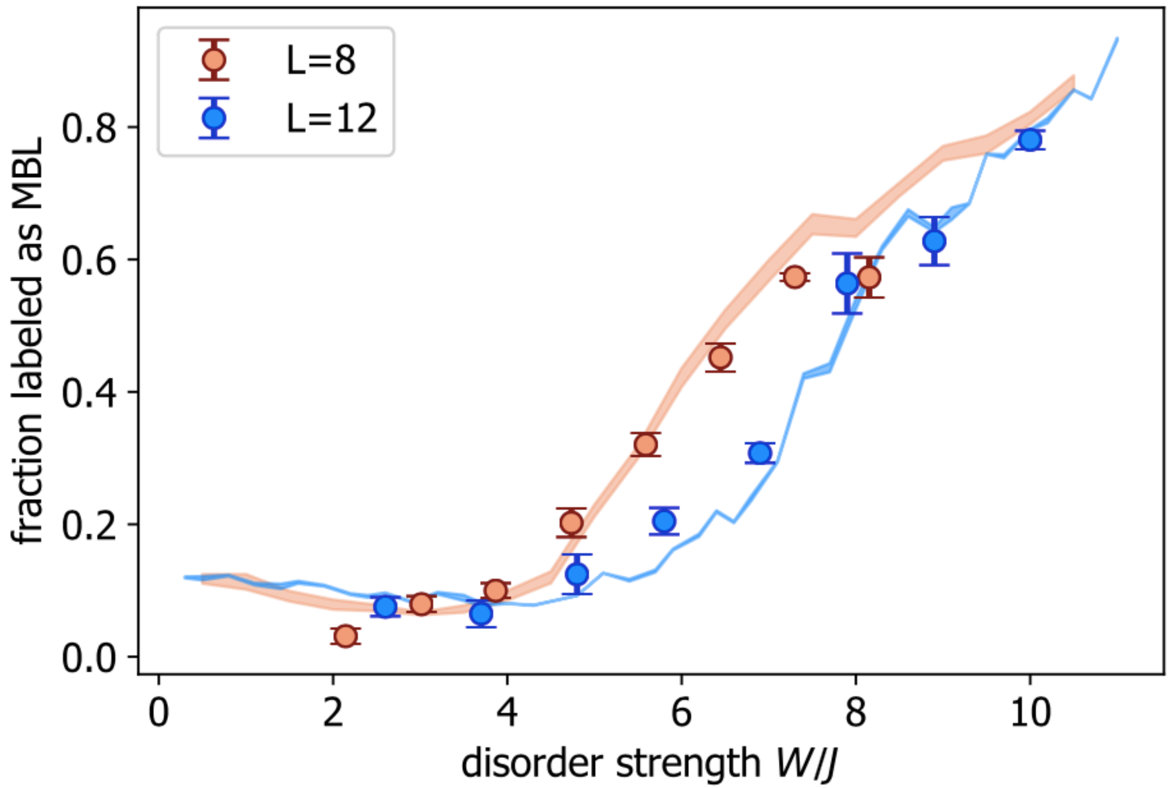
Cross entropy function

$$L_{CE} = y ln(a) + (1-y) ln(1-a) \longrightarrow L_{CE} = 2.3 \longrightarrow \frac{\partial L_{CE}}{\partial a} = 10$$

⇨ L_{CE} changes weights faster then L_{SE}

Analysis of non-equilibrium quantum states
Performance of the network

- Once the network reaches a high accuracy we put in experimental snapshots with different disorder strengths



A. Bohrdt et al. arXiv:2012.11586v1, 2020

Learning thermalization

Learning thermalization
The approach to thermal equilibrium

- Investigate dynamical evolution of the system
- Train neural network to distinguish equilibrium from dynamical behavior for each time step

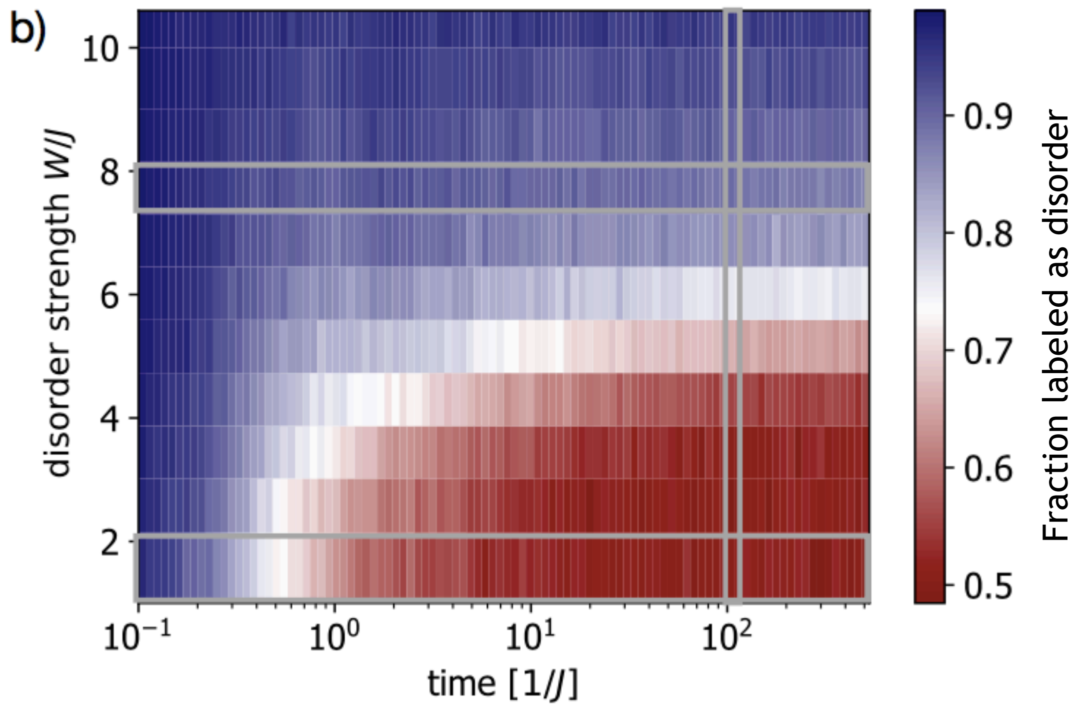
<u>Input:</u> time evolved state $\rightleftarrows$ thermal state

$\uparrow$

Matching energy density and temperature

Learning thermalization
The training data

- Input data obtained by exact diagonalization for different time steps
- Graph represents fraction labeled as disorder for different disorder strengths and times



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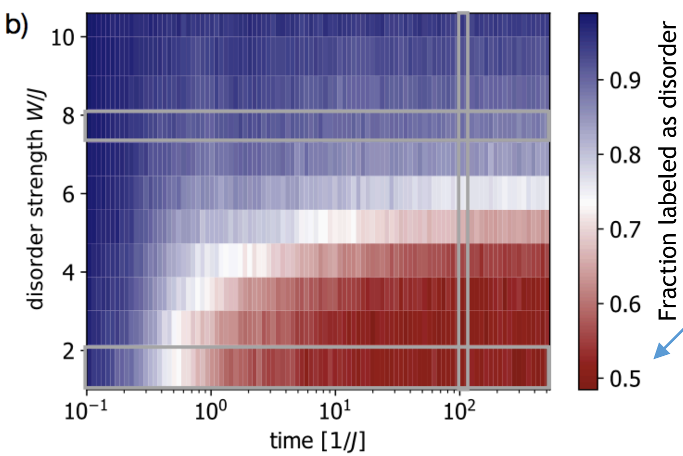
Learning thermalization
The training data

High W/J and long time scales	→	High disorder fraction
High W/J and short time scales	→	High disorder fraction
Low W/J and short time scales	→	High disorder fraction
Low W/J and long time scales	→	Low disorder fraction



for low disorder the network has an accuracy of 50% equivalent to guess between thermal and non-thermal state

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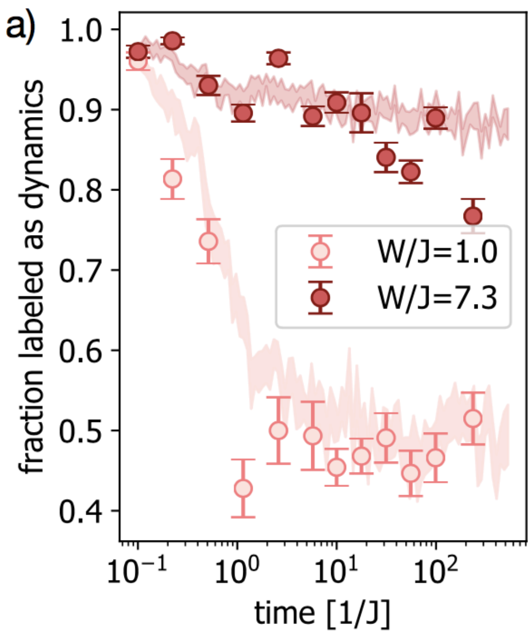
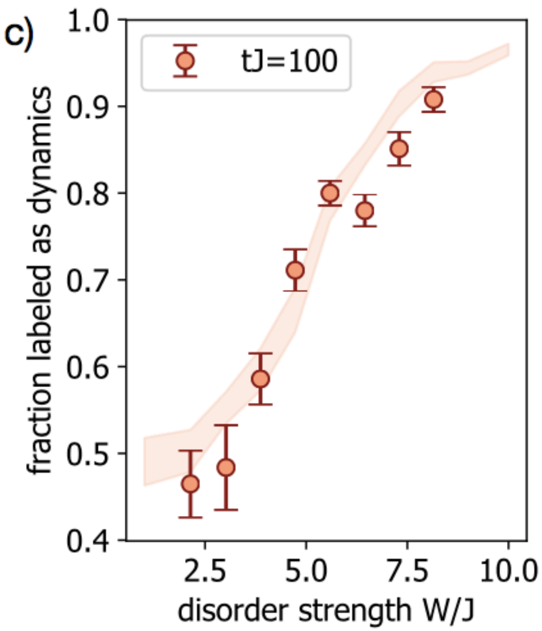
Learning thermalization
Performance of the network

- Network labeling performance for experimental data





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Finding exact transition

Finding exact transition
Confusion learning scheme

- Check if in a set of snapshots with different $0.3 < W/J < 11.0$ a W^* exists where data changes qualitatively
- Start by training network with a guessing W^*

$$W < W^* \xrightarrow{\text{label as}} \text{Phase A}$$

$$W > W^* \xrightarrow{\text{label as}} \text{Phase B}$$

Finding exact transition
Confusion learning scheme

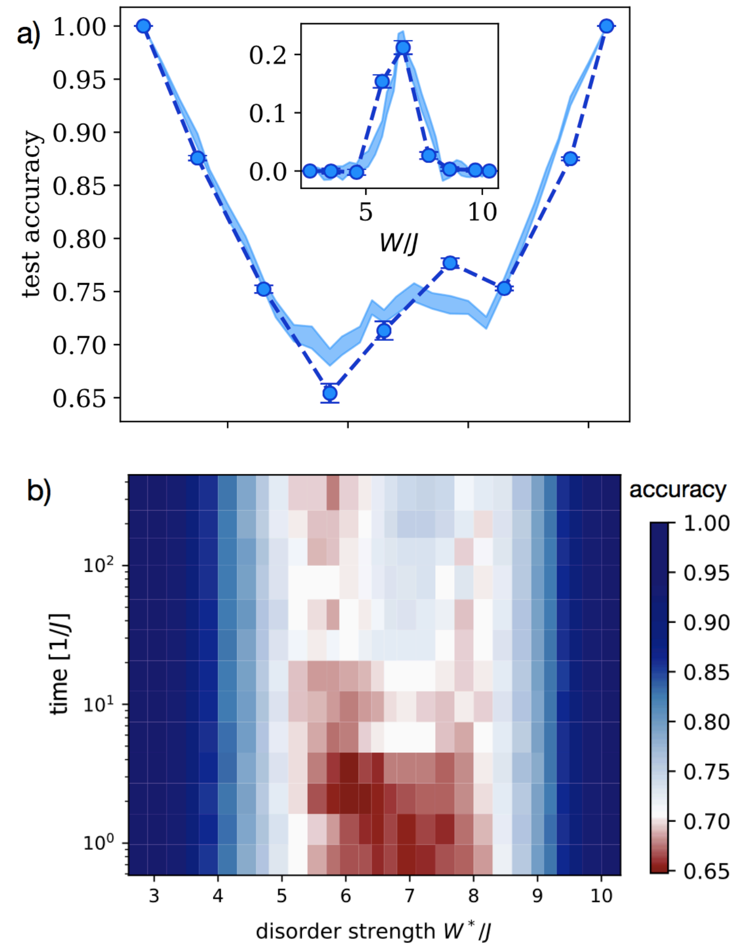
- Test the accuracy of the network with further experimental data assuming a qualitative change in the data
- We expect for different guesses different accuracies:

$W^*/J = 0.3$	$\rightarrow$	labeling as Phase B with high accuracy
$W^*/J = 11$	$\rightarrow$	labeling as Phase A with high accuracy
$W^* < W$	$\rightarrow$	Confusion occurs in labeling Phases
$W^* > W$	$\rightarrow$	Confusion occurs in labeling Phases
$W^* = W$	$\rightarrow$	High accuracy in assigning labels

Finding exact transition
Test accuracy function

- A phase transition occurs at W*/J = 7 (figure a)

- Phase transition remains on short time scales hidden



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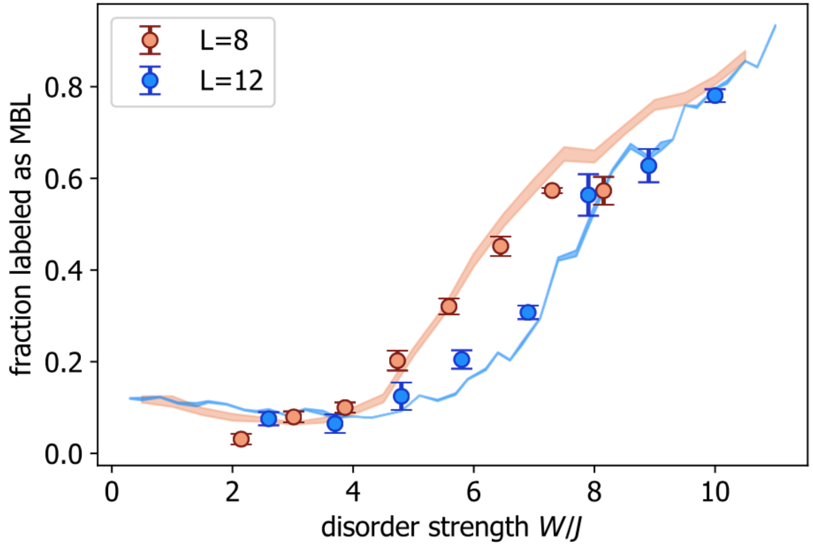
Summary

Summary
Analysis of non-equilibrium quantum states

- Machine learning techniques were used to to study non-equilibrium dynamics of ultra cold atoms
- Different lattice sizes were analyzed finding finite size effects
- Approach is not limited to system sizes



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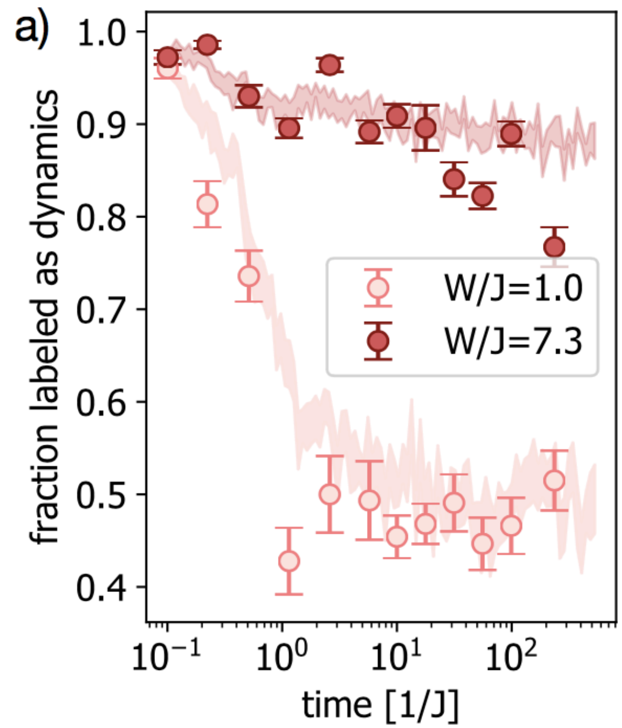
Summary
Learning thermalization

- The thermalization behavior was investigated time step wise enabling the recognition of MBL phases
- The method is applicable on a variety of models
- The method suffers from the need of numerically sampled snapshots



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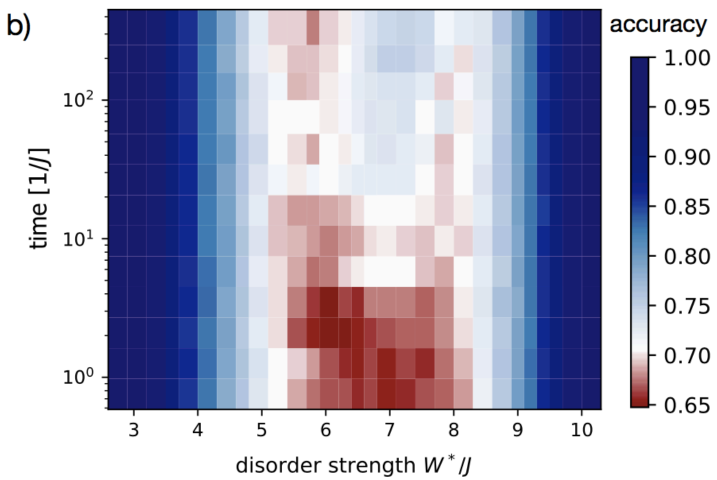
Summary
Finding exact transition

- An unsupervised learning scheme was applied to find the exact transition value (W/J = 7)
- The network seems to recognize observables able to identify a qualitative change in the data for long time scales
- The network recognized a transition without any bias



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Thank you!