Title: Quantum many-body dynamics in two dimensions with artificial neural networks

Speakers: Markus Heyl

Series: Machine Learning Initiative

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Abstract: In the last two decades the field of nonequilibrium quantum many-body physics has seen a rapid development driven, in particular, by the remarkable progress in quantum simulators, which today provide access to dynamics in quantum matter with an unprecedented control. However, the efficient numerical simulation of nonequilibrium real-time evolution in isolated quantum matter still remains a key challenge for current computational methods especially beyond one spatial dimension. In this talk I will present a versatile and efficient machine learning inspired approach. I will first introduce the general idea of encoding quantum many-body wave functions into artificial neural networks. I will then identify and resolve key challenges for the simulation of real-time evolution, which previously imposed significant limitations on the accurate description of large systems and long-time dynamics. As a concrete example, I will consider the dynamics of the paradigmatic two-dimensional transverse field Ising model, where we observe collapse and revival oscillations of ferromagnetic order and demonstrate that the reached time scales are comparable to or exceed the capabilities of state-of-the-art tensor network methods.

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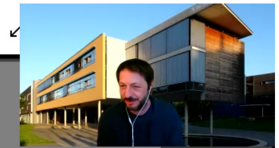
Quantum many-body dynamics in two dimensions with artificial neural networks



Markus Heyl

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PIQuIL Waterloo 03/05/2021

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University of Cologne

European Research Council

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JÜLICH

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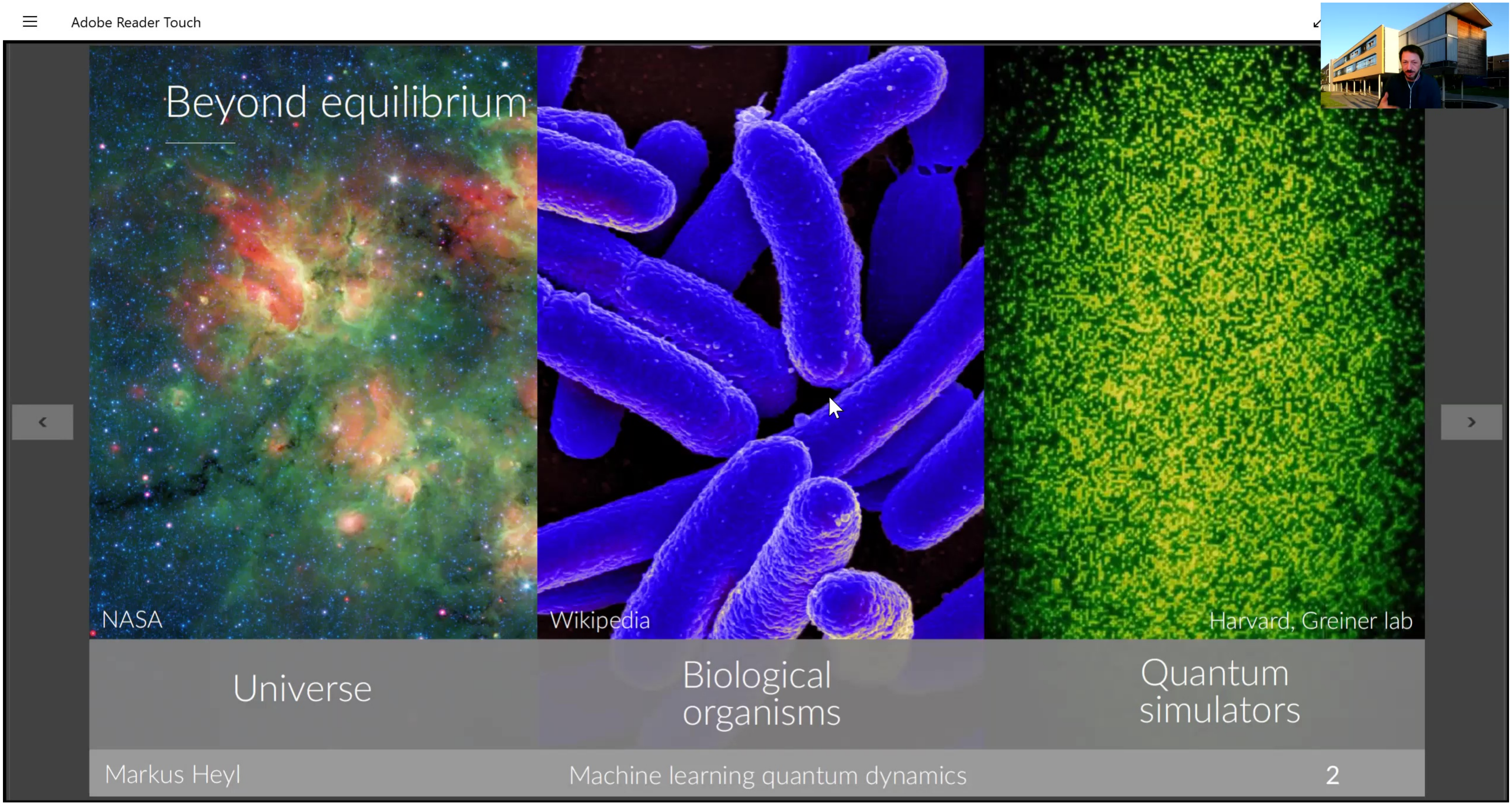
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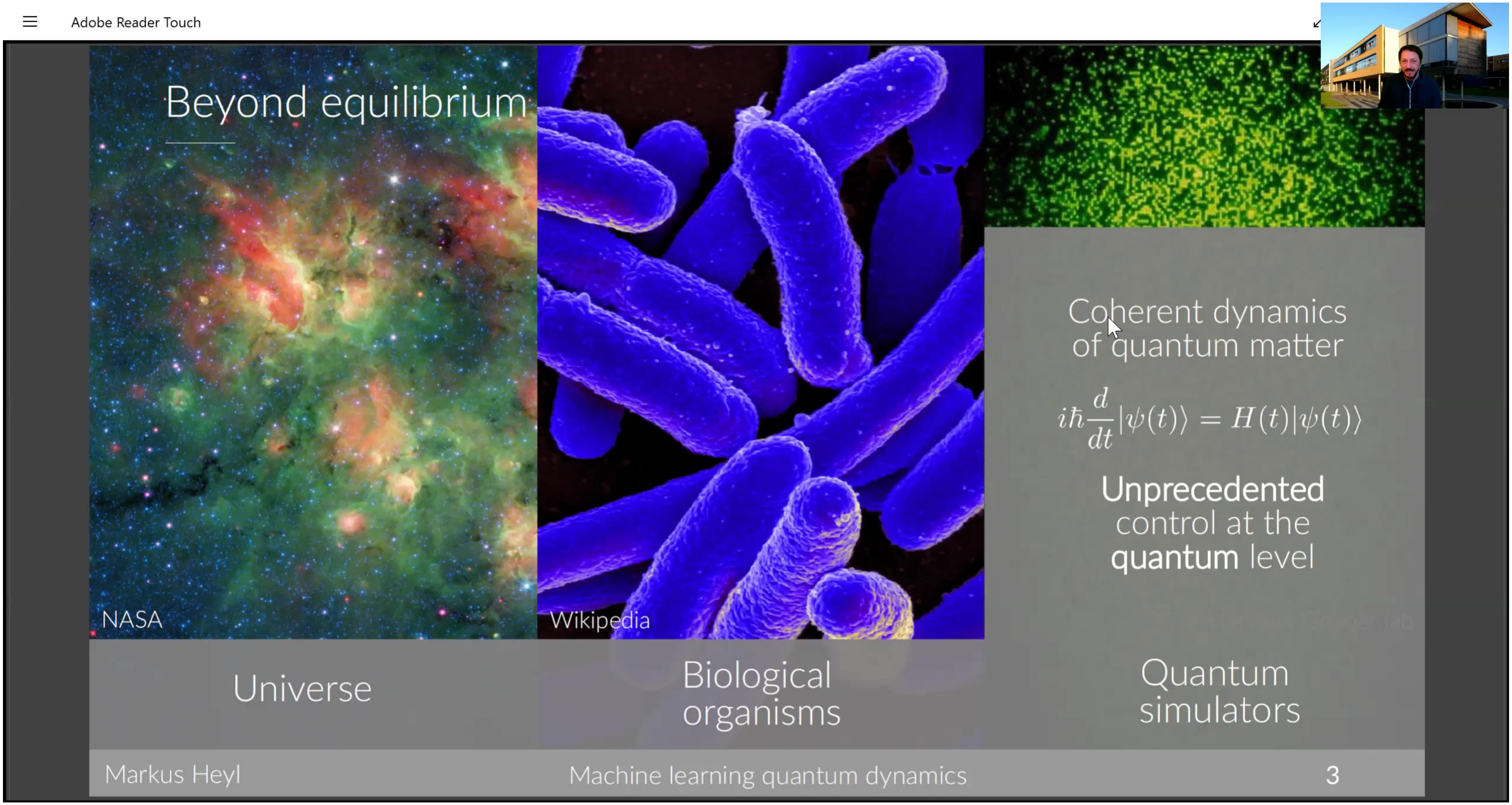
Beyond equilibrium
NASA
Wikipedia
Harvard, Greiner lab
Universe
Biological organisms
Quantum simulators
Markus Heyl
Machine learning quantum dynamics
2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Beyond equilibrium
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Coherent dynamics of quantum matter
$i\hbar\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$
Unprecedented control at the quantum level
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Biological organisms
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Markus Heyl
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3

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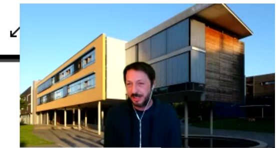

Dynamics in correlated quantum matter

Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

for many-body systems

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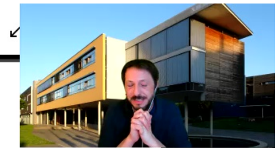

Outline

- Quantum dynamics in 2D: motivation and challenges
- Classical networks and artificial neural network wave functions
- The inversion problem: how to stabilize dynamics with neural networks
- Outlook

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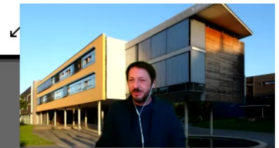
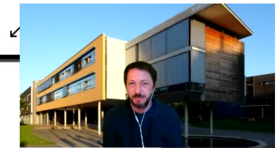


Quantum dynamics in 2D: motivation and challenges



Quantum Dynamics in 2D

Today: *key turning point* in theory and experiment

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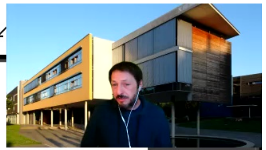
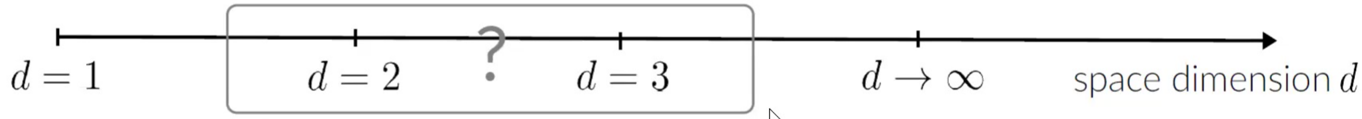


Quantum Dynamics in 2D

Today: *key turning point* in theory and experiment

Quantum simulators: Coherent dynamics of quantum matter in *2d*
Harvard, MPQ, Princeton, Paris,…

Theory: severe limitation for (numerically) exact methods



Tensor network methods →
Limited by entanglement
Review: Schollwöck '11

← Dynamical mean-field theory
Limited by spatial resolution
Review: Aoki '13

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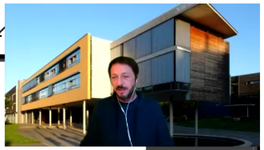

Dynamics in correlated quantum matter

Challenge: Hilbert space exponential

Quantum many-body state: $|\psi\rangle = \sum_s \psi(s)|s\rangle$ # amplitudes ~ 2^N (N spin-1/2's, fermions,...)

Exponential computational resources required
(without efficient compression)

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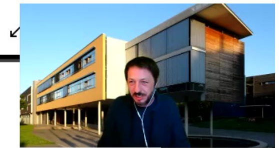

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Our approach

"Don't store. Generate on the fly."

$|s\rangle \longrightarrow$ Machine $\longrightarrow \tilde{\psi}(s) \approx \psi(s)$

sample with Monte Carleo (MC)

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Classical networks and artificial neural network wave functions

Classical networks

$|s\rangle$ → Classical network → $\tilde{\psi}(s,t) = e^{\mathcal{H}}$

Schmitt & MH SciPost '18

Effective classical Hamiltonian

- Structure obtained from cumulant expansion (around a classical limit)
- *Perturbatively* controlled
- Further *variationally* optimized

$$\mathcal{H}_{\text{eff}}(s,t) = h_0(s,t) + \epsilon h_1(s,t) + \epsilon^2 h_2(s,t) + \ldots$$

ϵ: small parameter

(similar to Jastrow or Huse & Elser wave functions)

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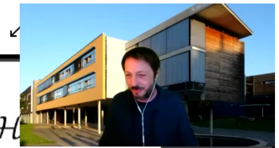

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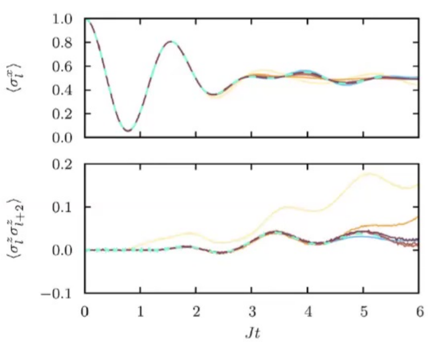
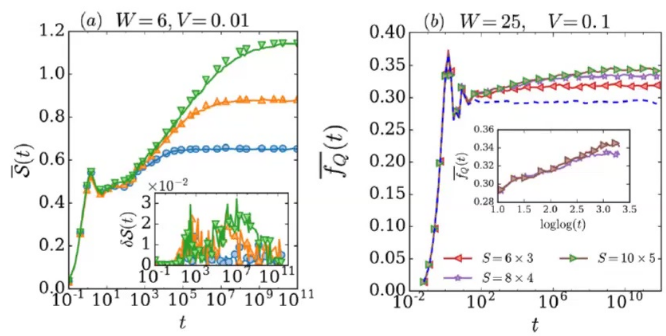
Successful for tailored problems

Quantum Ising 1D



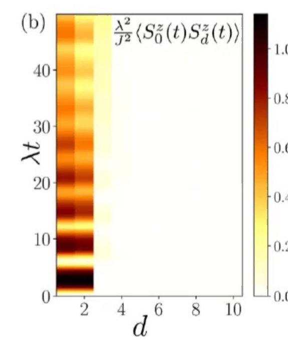
Aranda, MH, *et al*, arXiv '20

MBL



De Tomasi, Pollmann, & MH PRB (R) '19

Quantum link model in 2D



Karpov, MH, *et al*, arXiv '20

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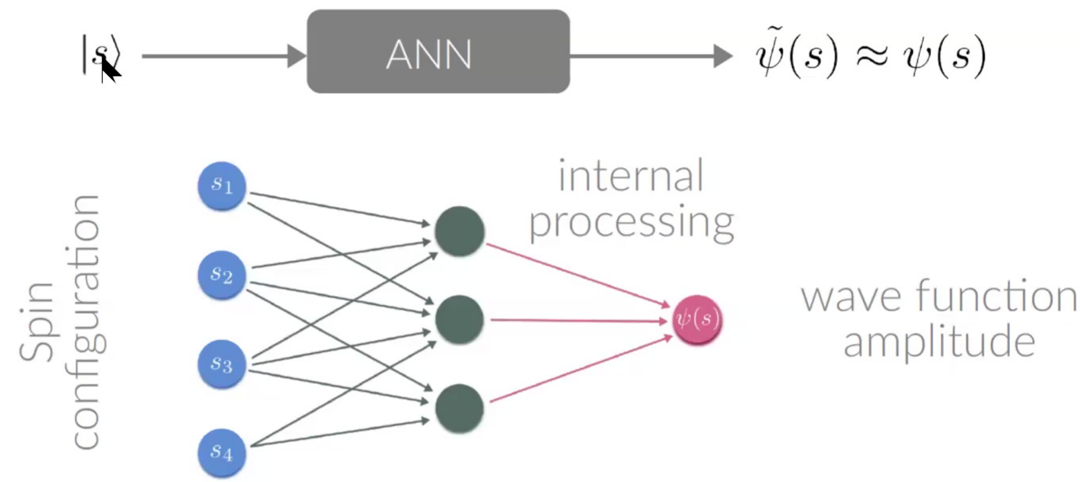
Encoding quantum states in artificial neural networks (ANN)



Enabling idea: ANNs ***universal function approximators***

$\rightarrow$ *Any* quantum state can be encoded in a (sufficiently large) ANN

Carleo & Troyer Science '17

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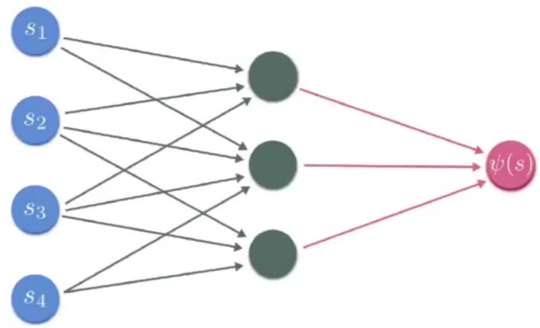
Encoding quantum states in artificial neural networks (ANN)



Enabling idea: ANNs *universal function approximators*

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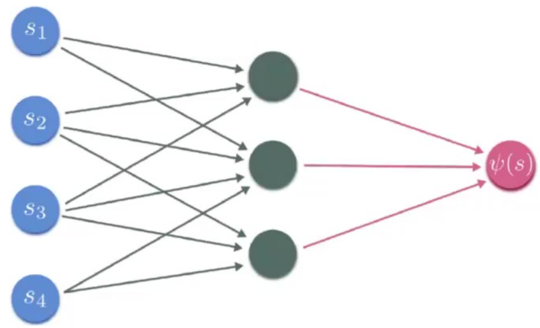

Enabling idea: ANNs *universal function approximators*

ANN is not just a black box → Numerically exact approach

Convergence parameter: size of ANN

Complexity of algorithm: poly(size of ANN, system size)

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Challenging for nonequilibrium dynamics

Results in the literature: limitations
(either in system size, time,...)

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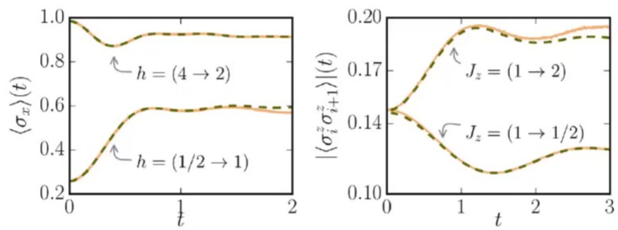

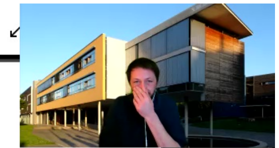

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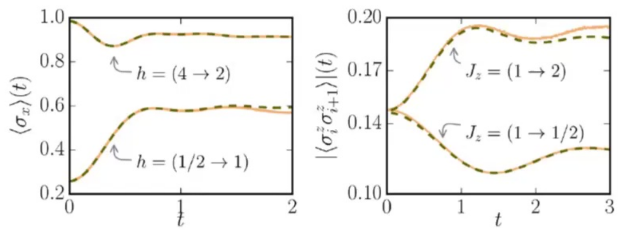
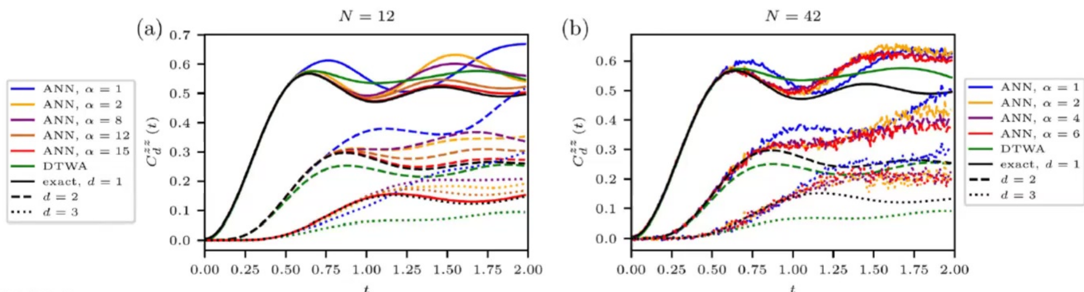
Carleo & Troyer Science '17

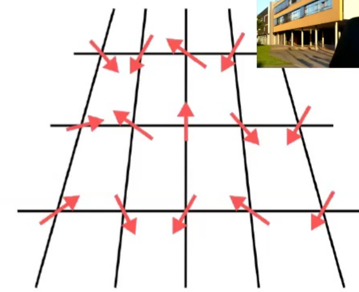




Systematic discrepancy even for increasing size of net

Czischek *et al* PRB '18

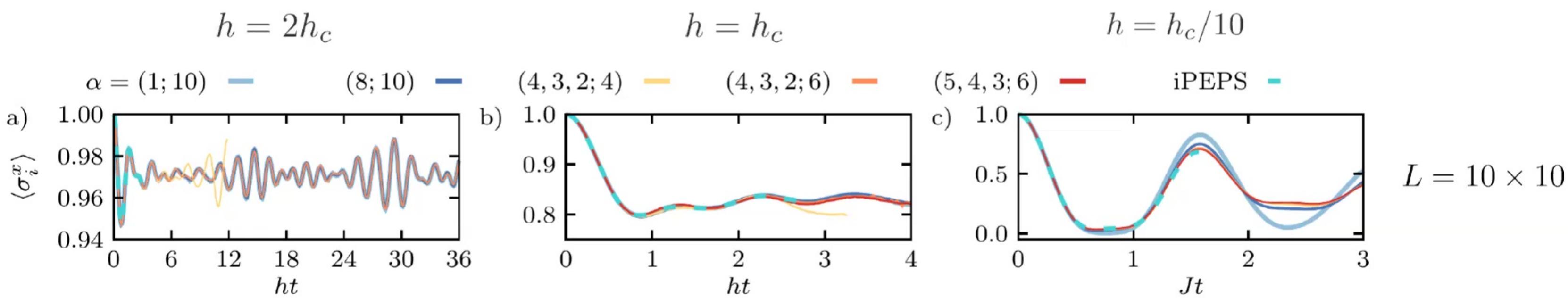
Overcoming the challenges



2D transverse-field Ising model $$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_j \sigma_j^x$$

Nonequilibrium quantum quench: $|\psi_0\rangle = |\rightarrow\rangle \implies |\psi_0(t)\rangle = e^{-iHt}|\psi_0\rangle$

M. Schmitt & **MH** PRL '20



iPEPS data from Czarnik *et al.* PRB '19

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The inversion problem: how to stabilize dynamics with neural networks

Markus Heyl Machine learning quantum dynamics 21

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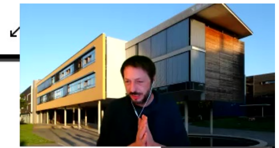
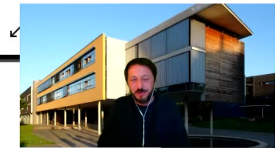


The setup

Quantum many-body wave function

$$|\psi\rangle = \sum_s \psi(s)|s\rangle$$



The setup

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$$|\psi\rangle = \sum_s \psi(s)|s\rangle$$

Solving the dynamics

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle, \quad |\psi(t)\rangle = \sum_s \psi(s,t)|s\rangle$$

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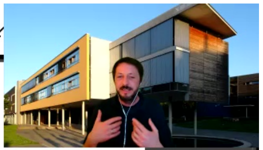

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Quantum many-body wave function

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Solving the dynamics

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle, \quad |\psi(t)\rangle = \sum_s \psi(s,t)|s\rangle$$

Approximate time-evolved state by variational wave function

$$|\psi(t)\rangle \approx |\psi_{\eta(t)}\rangle = \sum_s \psi_{\eta(t)}(s)|s\rangle$$

Goal: choose variational parameters *optimally*. How?

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Time-dependent variational principle

Do (*infinitesimal*) step

$$|\psi_{\eta(t)}\rangle \mapsto e^{-iH\Delta t}|\psi_{\eta(t)}\rangle$$

Is now out of the variational subspace

Time-dependent variational principle

Do (*infinitesimal*) step

$$|\psi_{\eta(t)}\rangle \mapsto e^{-iH\Delta t}|\psi_{\eta(t)}\rangle$$

Is now out of the variational subspace

Project back and identify a **new optimal** set of variational parameters

$$F_{\eta'} = |\langle\psi_{\eta'}|e^{-iH\Delta t}|\psi_{\eta(t)}\rangle| \quad \Longrightarrow \quad \sup_{\eta'} F_{\eta'}$$

For an infinitesimal time step: *Taylor expansion*

$$\eta' = \eta + \Delta\eta, \quad e^{-iH\Delta t} = 1 - iH\Delta t - \frac{1}{2}H^2\Delta t + \ldots$$

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Time-dependent variational principle

Quantum dynamics → Nonlinear classical **ODE** for *network weights* η_k

$$S_{k,k'}\dot{\eta}_{k'} = F_k$$

$$S_{k,k'} = \langle\langle O_k^* O_{k'} \rangle\rangle_c \qquad F_k = -i\langle\langle O_k^* E_{\text{loc}} \rangle\rangle_c$$

$$O_k(s) = \frac{\partial \ln \psi_\eta(s)}{\partial \eta_k} \qquad E_{\text{loc}}(s) = \sum_{s'} \langle s|H|s'\rangle \frac{\psi_\eta(s')}{\psi_\eta(s)}$$

When solved exactly: prescription to follow the *minimum* in variational manifold **step by step**

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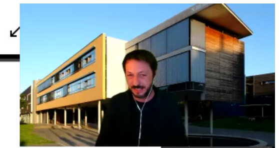

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$$S_{k,k'} = \langle\langle O_k^* O_{k'} \rangle\rangle_c \rightarrow S_{k,k'} \dot{\eta}_{k'} = F_k \leftarrow F_k = -i \langle\langle O_k^* E_{\text{loc}} \rangle\rangle_c$$

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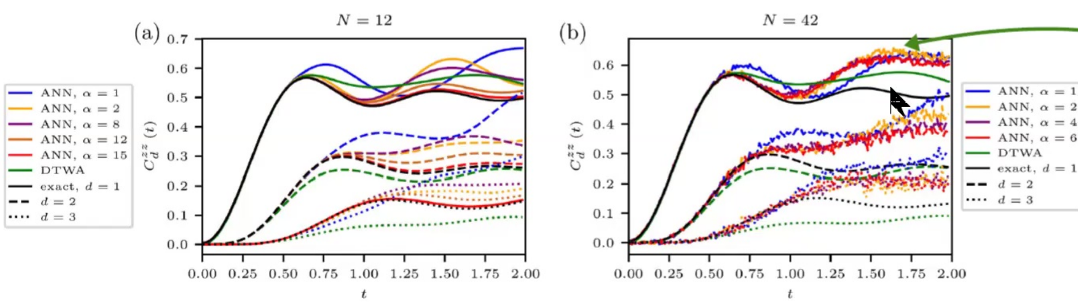
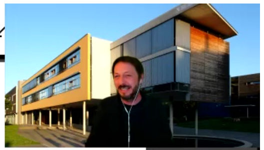


Systematically following a *local* minimum



Key solution: properly account for noisy estimates

$$S\dot{\eta} = F \quad \Rightarrow \quad \dot{\eta} = S^{-1}F$$

M. Schmitt & **MH** PRL '20

Problem: S **not** invertible...

→ Pseudo-inverse: threshold on singular values

But: We do MC and there is *noise everywhere*
(also in the singular values)

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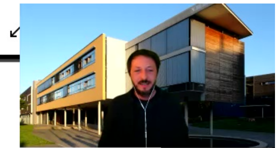

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Problem: S not invertible...

→ Pseudo-inverse: threshold on singular values

But: We do MC and there is *noise everywhere*
(also in the singular values)

Solution: Represent TDVP in the *diagonal basis* of the S matrix

$$S_{k,k'}\dot{\eta}_{k'} = F_k \quad \longrightarrow \quad \sigma_k^2 \dot{\tilde{\eta}}_k = \langle\langle Q_k^* E_{loc} \rangle\rangle_c \equiv \rho_k$$

$$S_{k,k'} = V_{k,l}\sigma_l^2 (V^\dagger)_{l,k'}, \; Q_k = (V^\dagger)_{k,k'} O_k,$$

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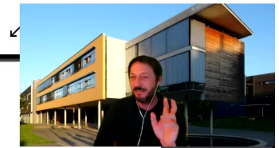


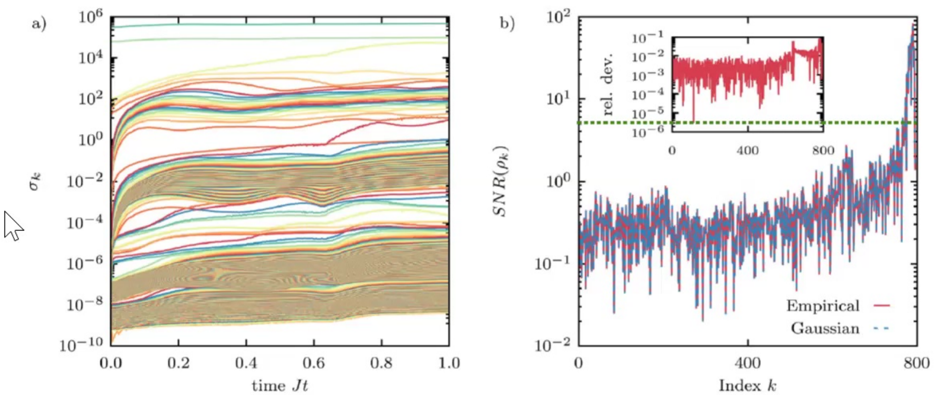
Key solution: properly account for noisy estimates

$$\sigma^2 \dot{\tilde{\eta}} = \rho$$

M. Schmitt & **MH** PRL '20

Noise *independent* of signal strength

$$SNR(\sigma_k) = \sqrt{N_{MC}/2}$$



Signal to noise ratio can vary over orders of magnitude

$$SNR(\rho_k) = \sqrt{\frac{N_{MC}}{1 + \frac{\sigma_k^2}{\rho_k^2}\mathrm{Var}(H)}}$$

New **regularization** scheme for inversion: SNR threshold

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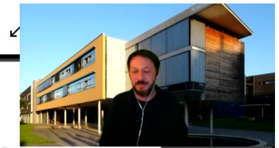

Overcoming the challenges

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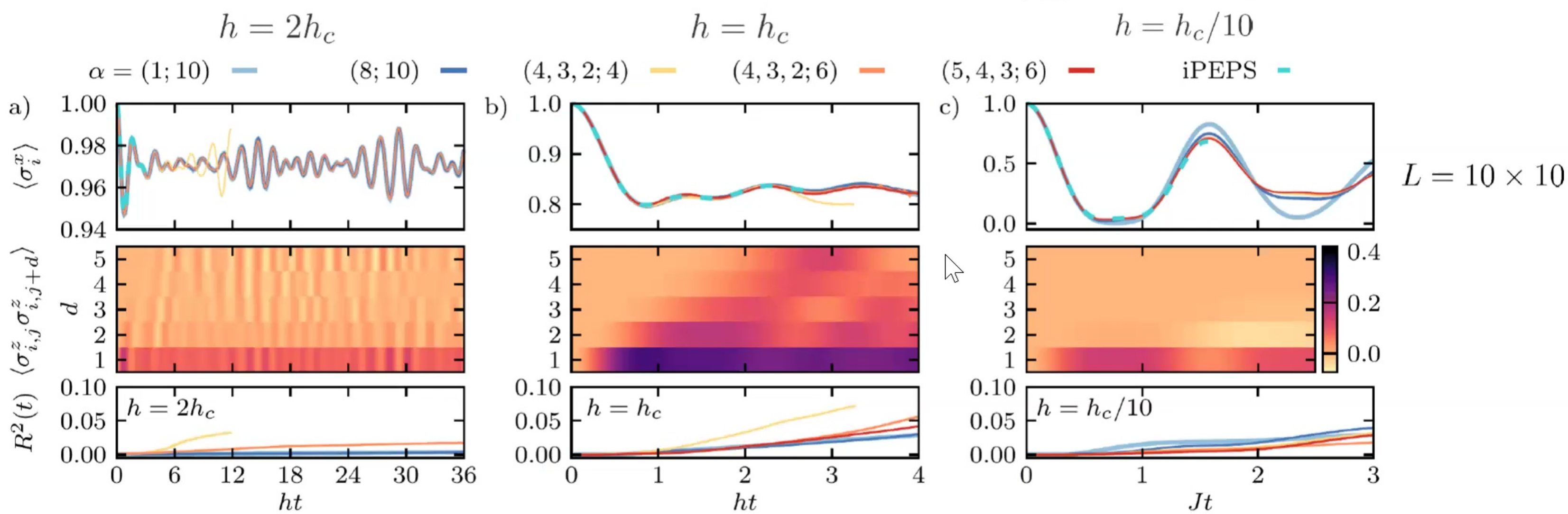
Quantum quenches in the 2D transverse-field Ising model

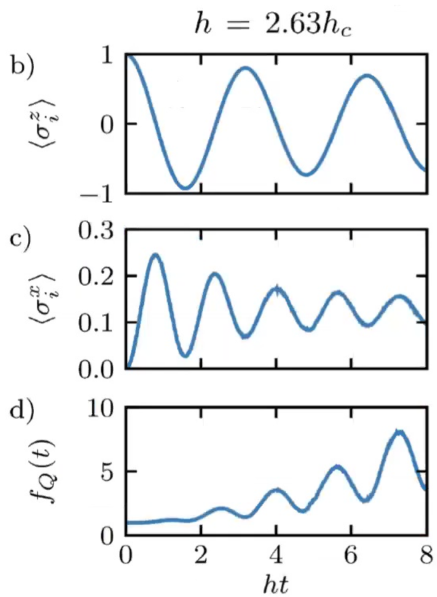
$$|\psi_0\rangle = |\rightarrow\rangle \quad \Longrightarrow \quad |\psi_0(t)\rangle = e^{-iHt}|\psi_0\rangle, \qquad H = -J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z - h\sum_j \sigma_j^x$$



iPEPS data from Czarnik *et al.* PRB '19

Collapse and revival oscillations in the 2D Ising model

$$|\psi_0\rangle = |\uparrow\rangle \implies |\psi_0(t)\rangle = e^{-iHt}|\psi_0\rangle$$



Order parameter
→ decay and revival of long-range order

Transverse magnetization
→ Buildup of thermal magnetization profile

Quantum Fisher information density
→ significant *multipartite entanglement*

$$f_Q(t) = \frac{1}{N}\sum_{i,j}\langle\sigma_i^z\sigma_j^z\rangle_c$$

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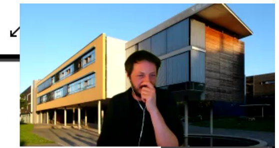
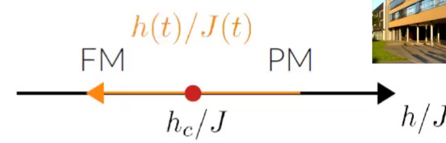


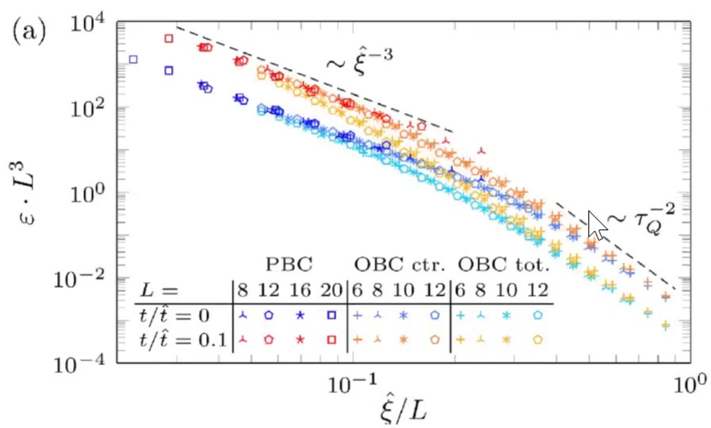
Outlook

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_j \sigma_j^x$$



Kibble-Zurek mechanism in 2D transverse-field Ising model

(together with M. Schmitt, M. Rams, J. Dziarmaga, W. Zurek)



→ room for exploring yet inaccessible regimes with ANNs

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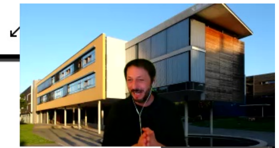

Summary

Powerful tool to describe nonequilibrium dynamics in 2D

- Competitive with (or even superior to) tensor networks
- Increasing system size or time at moderate polynomial costs
- Current limitations: still instabilities
- Not (so much) limited by network size (expressivity)