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

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European Research Council
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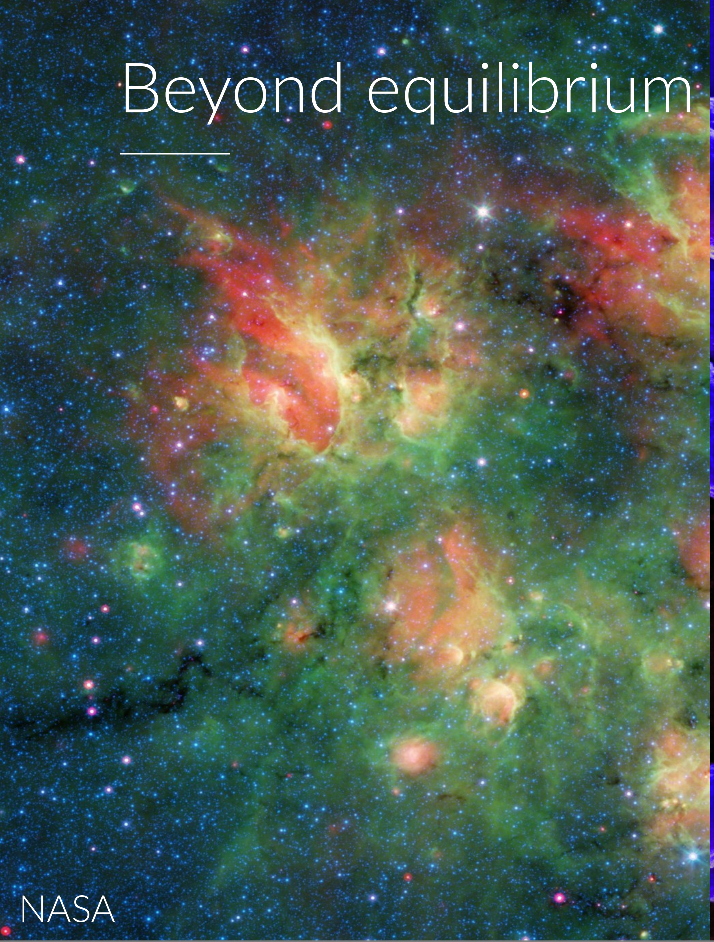
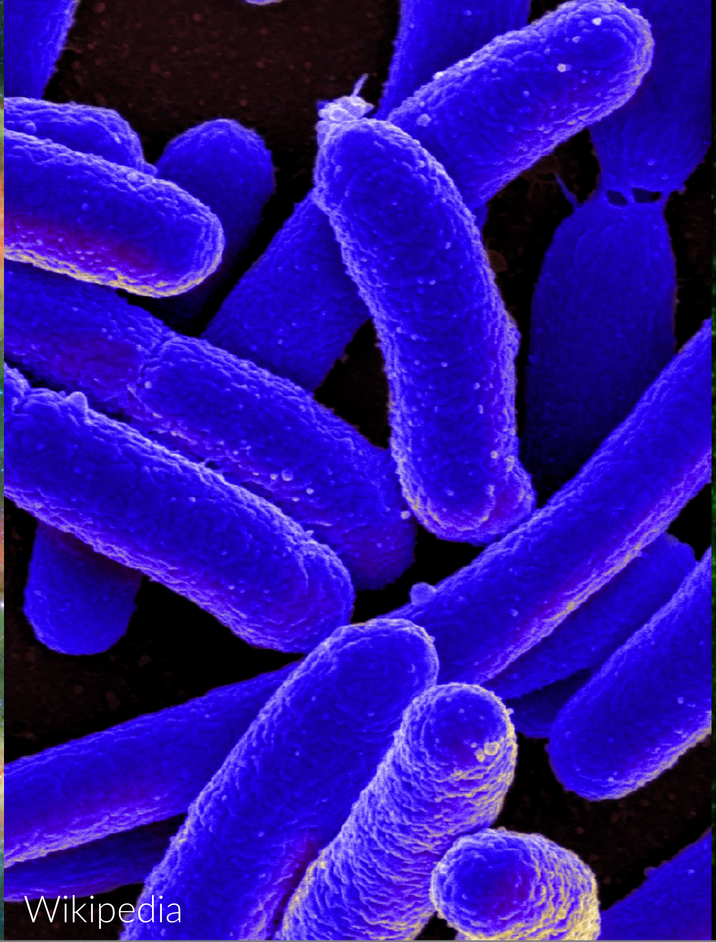
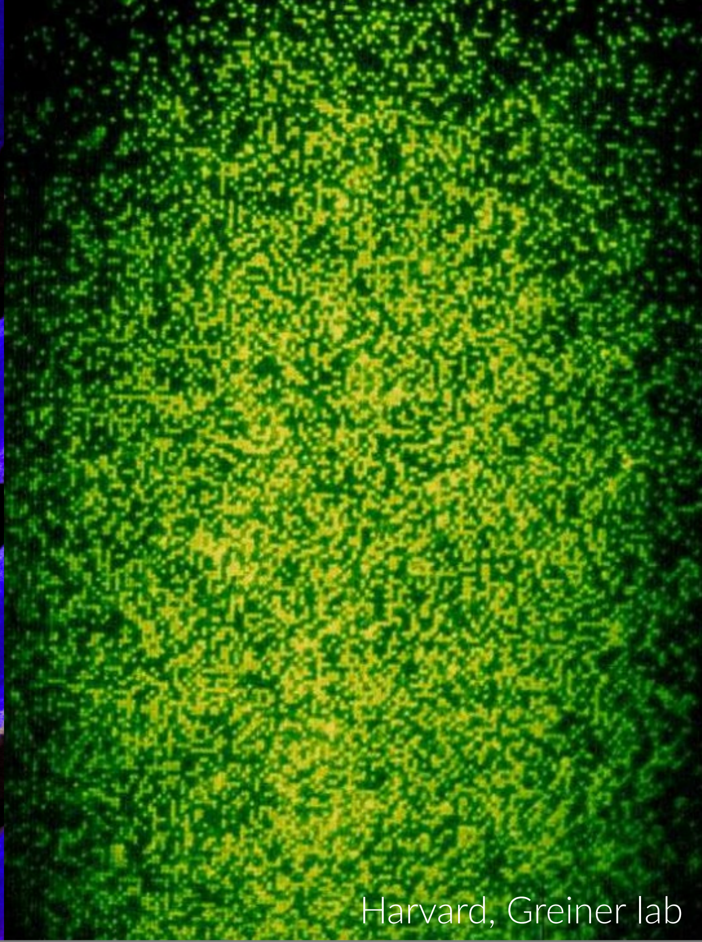
Beyond equilibrium



Universe

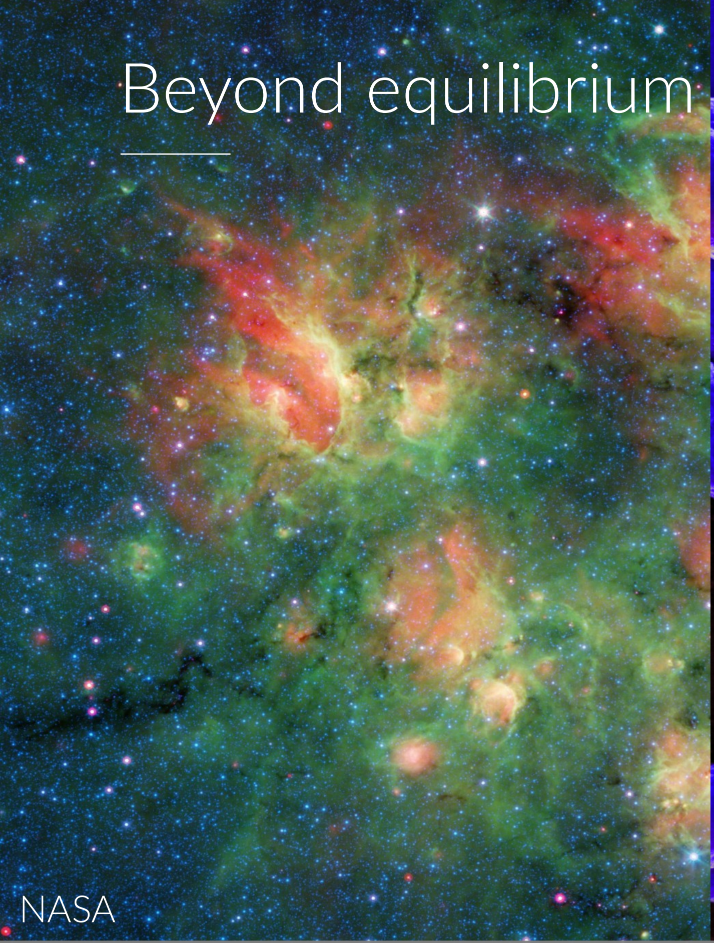


Biological organisms

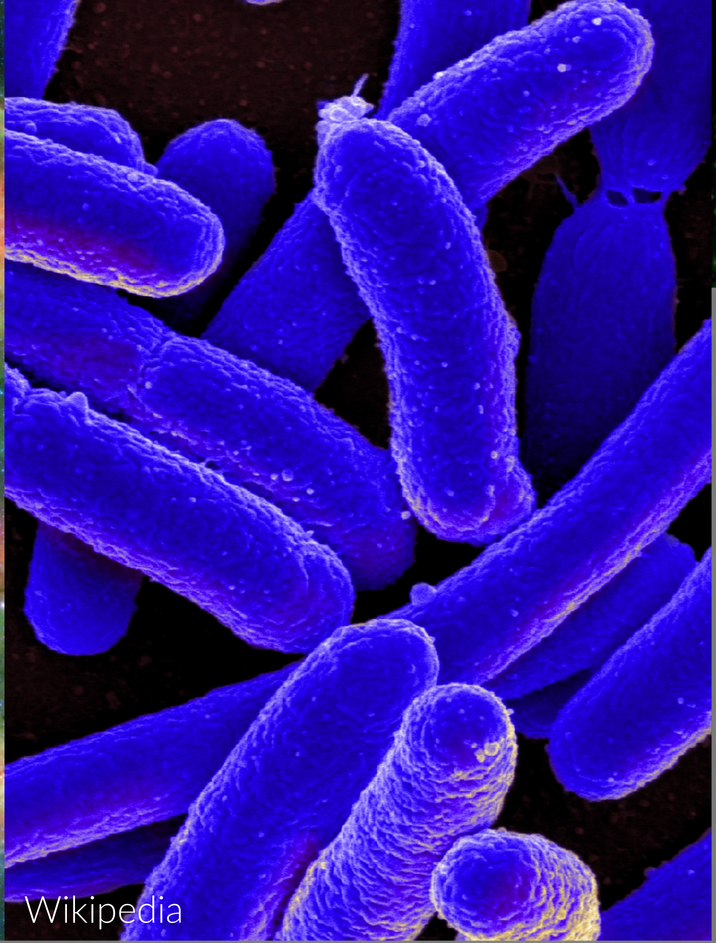


Quantum simulators

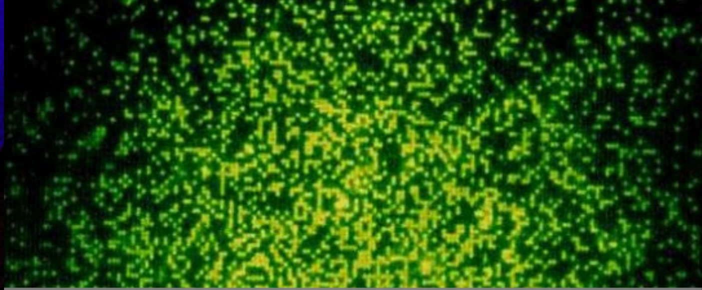
Beyond equilibrium


NASA

Universe


Wikipedia

Biological organisms



Coherent dynamics of quantum matter

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

Unprecedented control at the **quantum** level

Harvard, Greiner lab

Quantum simulators

Dynamics in correlated quantum matter

Schrödinger equation

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

for many-body systems

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

Quantum dynamics in 2D: motivation and challenges

Quantum Dynamics in 2D

Today: *key turning point* in theory and experiment

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Quantum simulators: Coherent dynamics of quantum matter in *2d*

Harvard, MPQ, Princeton, Paris,...

Theory: severe limitation for (numerically) exact methods

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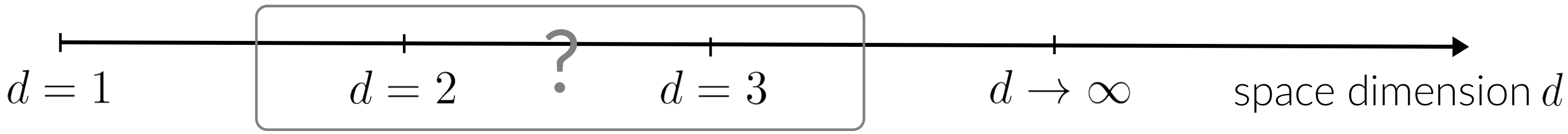

Tensor network methods $\longrightarrow$
Limited by entanglement
Review: Schollwöck '11

$\longleftarrow$ Dynamical mean-field theory
Limited by spatial resolution
Review: Aoki '13

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)

Dynamics in correlated quantum matter

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Exponential **computational** resources **required**
(without efficient compression)

Our approach

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

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

sample with Monte Carleo (MC)

Classical networks and artificial neural network wave functions

Classical networks

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

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)

Classical networks

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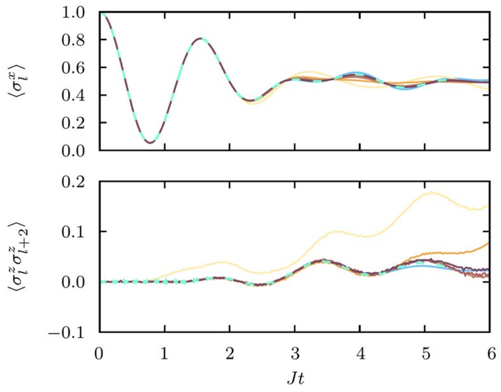
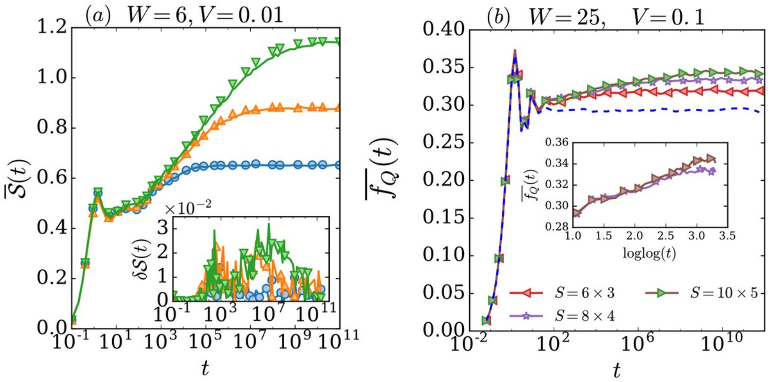
Successful for **tailored** problems

Quantum Ising 1D



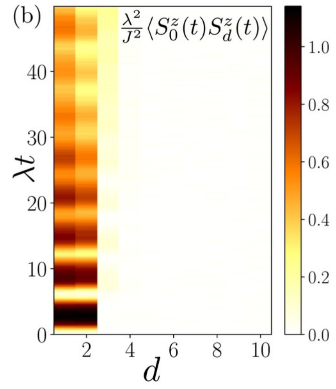
Aranda, **MH**, *et al*, arXiv '20

MBL



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

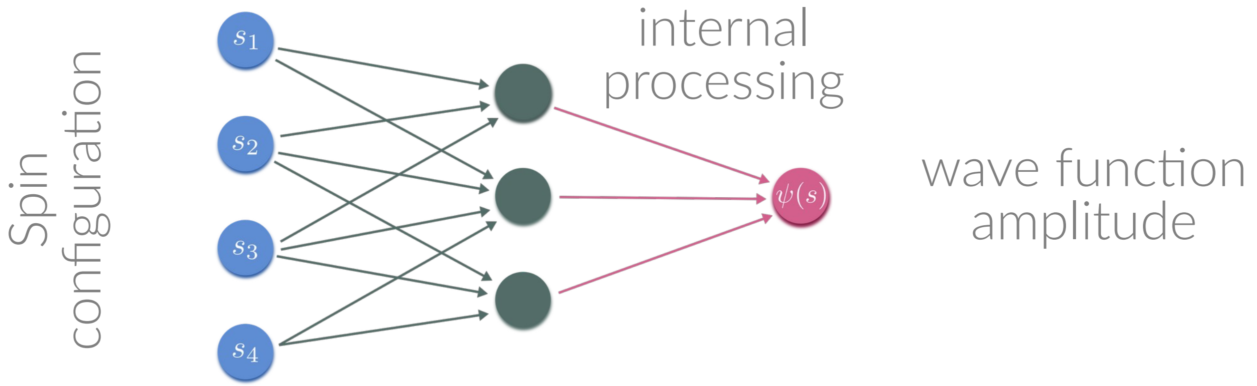
Quantum link model in 2D



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

Encoding quantum states in artificial neural networks (ANN)

$$|s\rangle \longrightarrow \boxed{\text{ANN}} \longrightarrow \tilde{\psi}(s) \approx \psi(s)$$

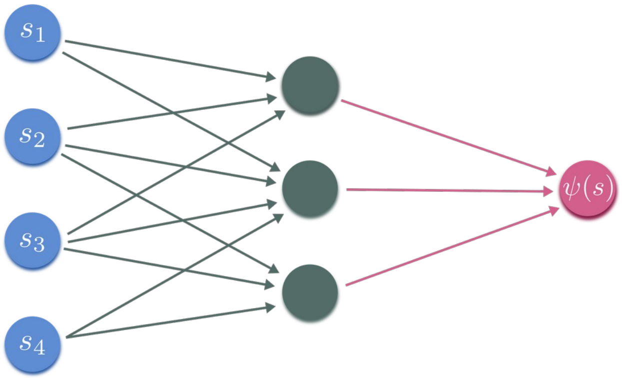


Enabling idea: ANNs *universal function approximators*

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

Carleo & Troyer Science '17

Encoding quantum states in artificial neural networks (ANN)



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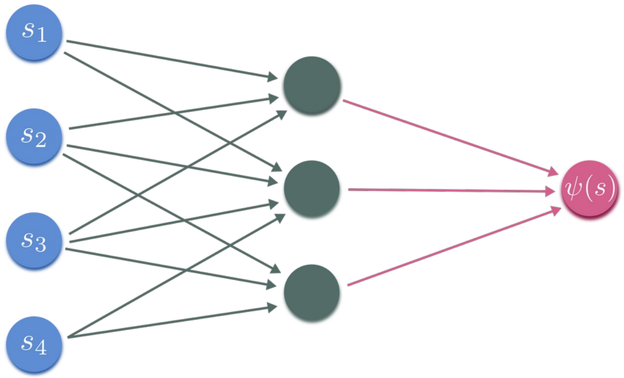


Enabling idea: ANNs *universal function approximators*

ANN is not just a black box → Numerically exact approach

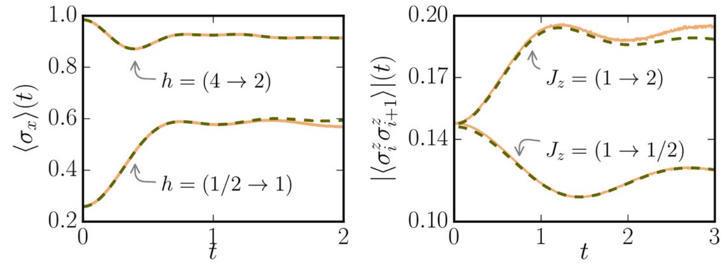
Convergence parameter: size of ANN

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

Challenging for nonequilibrium dynamics

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

Carleo & Troyer Science '17



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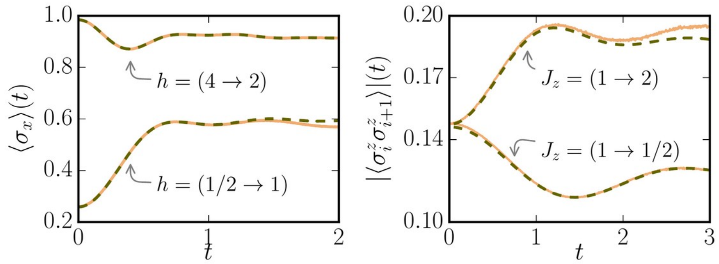
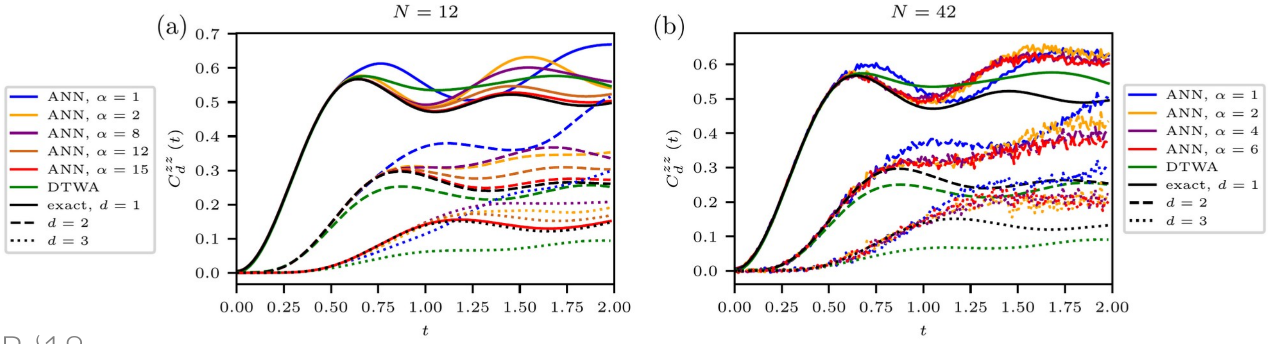
Carleo & Troyer Science ‘17

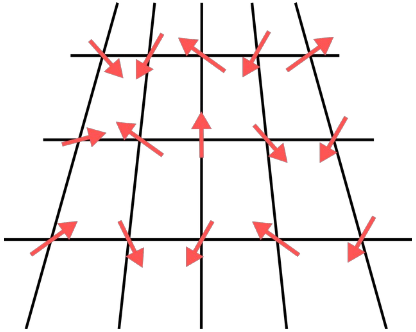




Systematic discrepancy even for increasing size of net

Czischek *et al* PRB ‘18

Overcoming the challenges

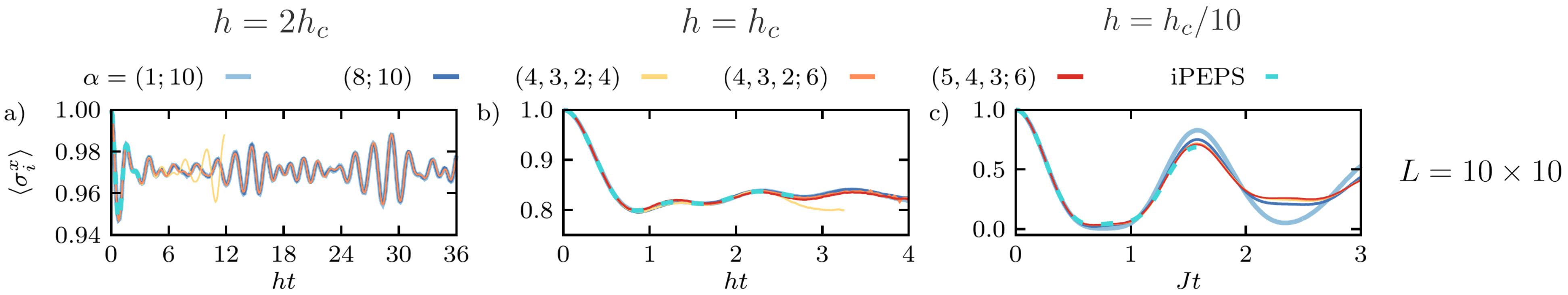


2D transverse-field Ising model

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

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

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



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

The inversion problem: how to stabilize dynamics with neural networks

The setup

Quantum many-body wave function

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Solving the dynamics

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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?

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

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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*

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

Time-dependent variational principle

Quantum dynamics $\rightarrow$ Nonlinear classical ODE for *network weights* η_k

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

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

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

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

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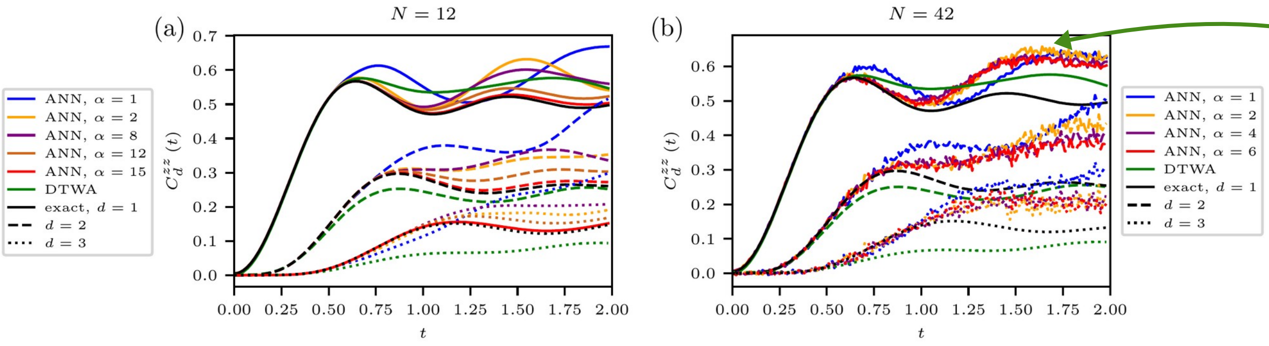

Systematically following a *local* minimum

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…

$\rightarrow$ Pseudo-inverse: threshold on singular values

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

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

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

$\rightarrow$ 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

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

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

Key solution: properly account for noisy estimates

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

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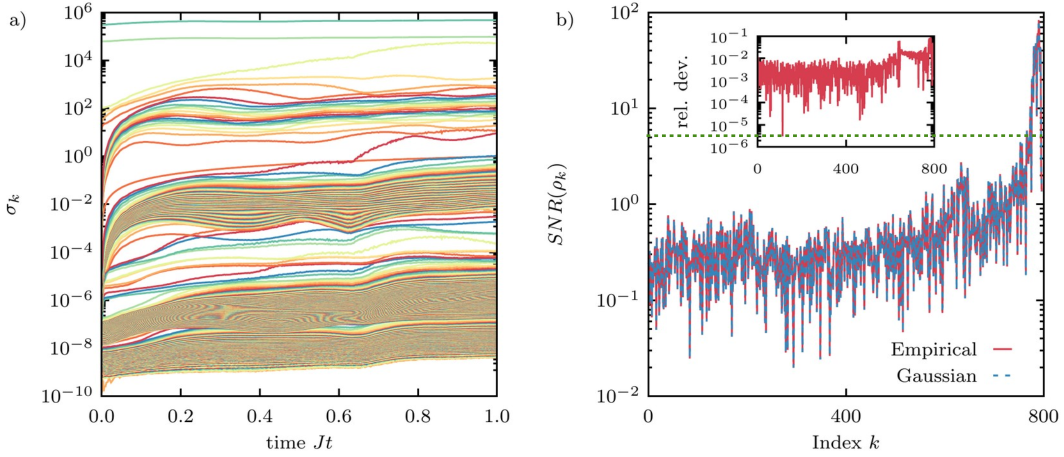
Noise *independent* of signal strength

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



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

Overcoming the challenges

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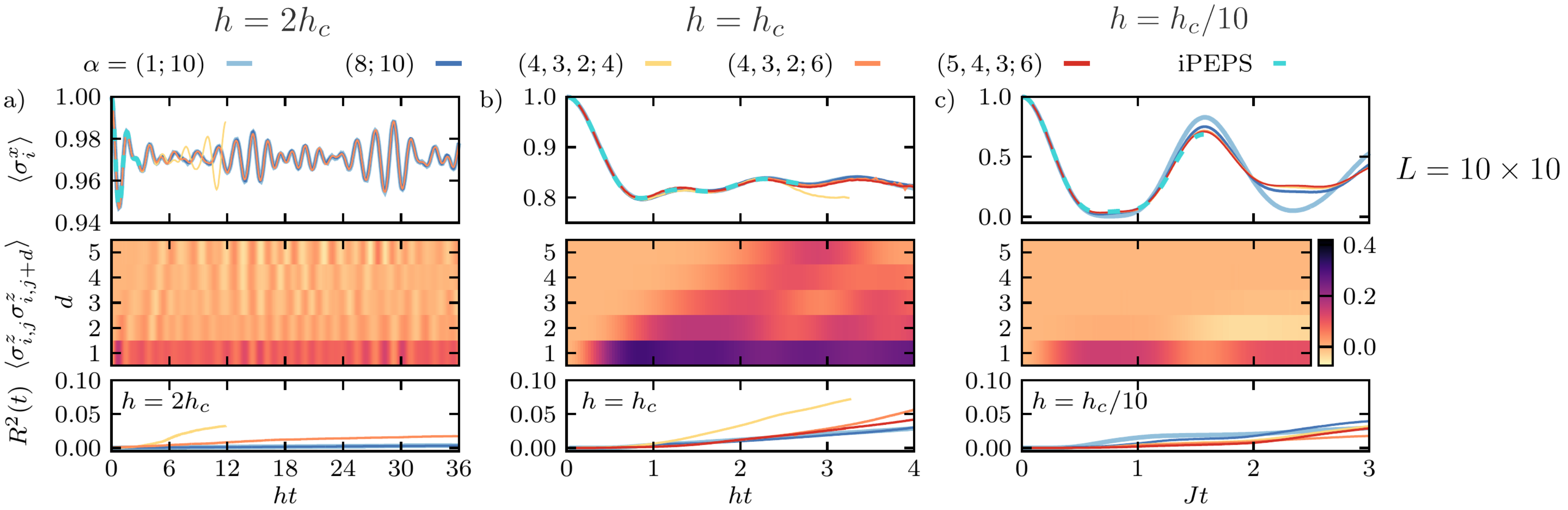
Quantum quenches in the 2D transverse-field Ising model

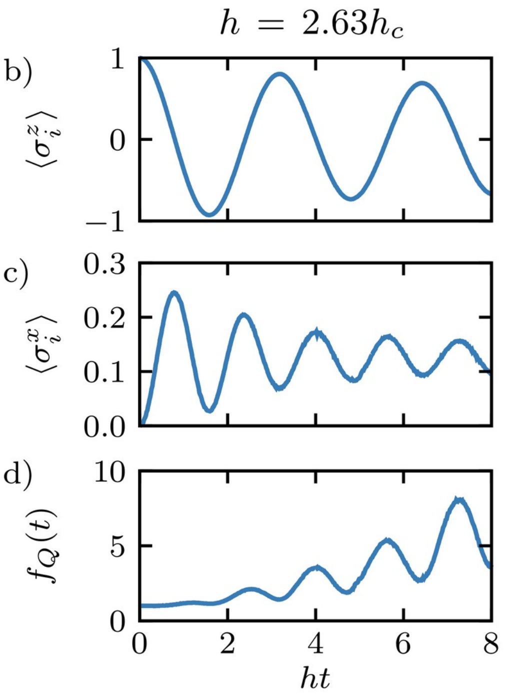
$$|\psi_0\rangle = |\rightarrow\rangle \quad \Longrightarrow \quad |\psi_0(t)\rangle = e^{-iHt}|\psi_0\rangle, \qquad H = -J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z - h\sum_j \sigma_j^x$$



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

Collapse and revival oscillations in the 2D Ising model

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



Order parameter
→ decay and revival of long-range order

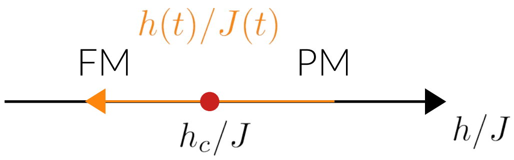
Transverse magnetization
→ Buildup of thermal magnetization profile

Quantum Fisher information density
→ significant *multipartite entanglement*

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

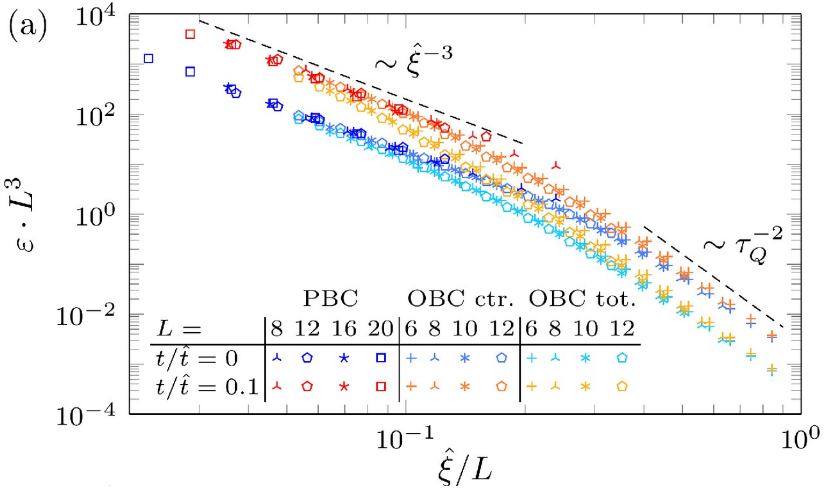
Outlook

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



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

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

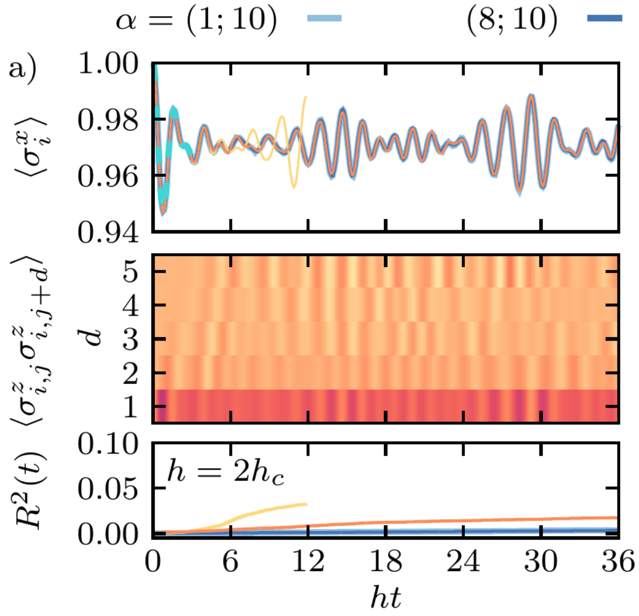


→ room for exploring yet inaccessible regimes with ANNs

Summary

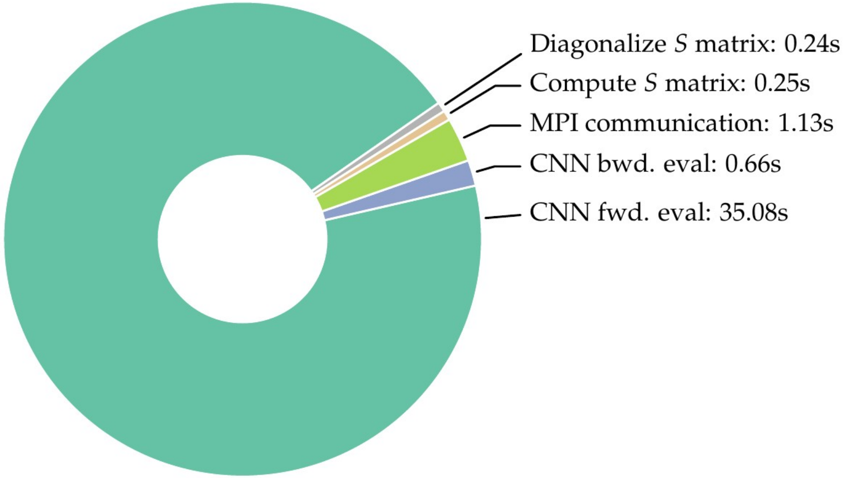
Powerful tool to describe nonequilibrium dynamics in 2D

- 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)



Computational resources

Distribution of compute time for one time step on 40 NVIDIA Tesla V100 GPUs



$$N_{MC} = 5 \cdot 10^5 \qquad N = 100$$

Overall complexity: $\mathcal{O}(N_{MC} \times \max(N^2, P) \times P)$