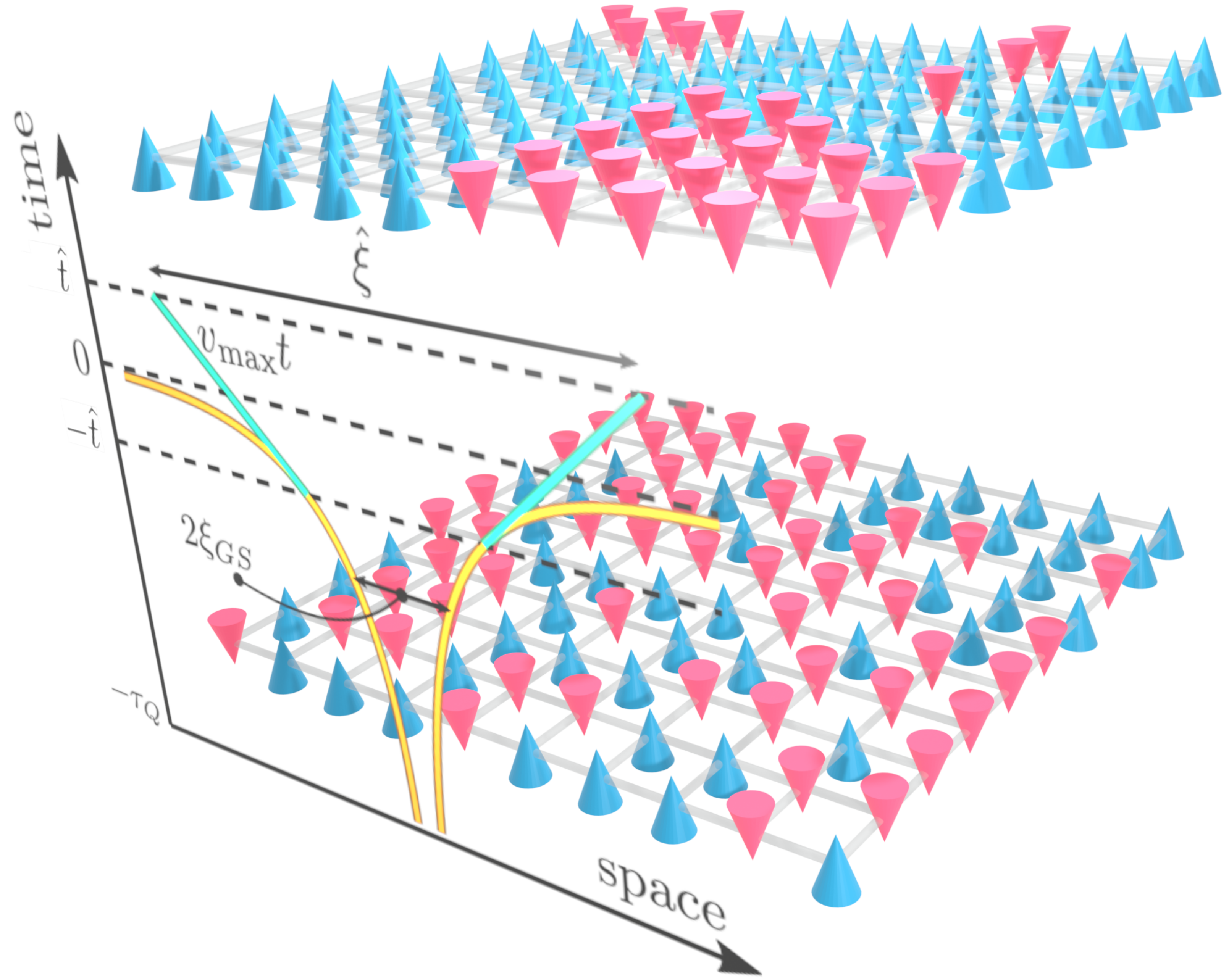
Revealing dynamical universality with neural quantum states



Markus Schmitt

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Mar 29, 2022 — AMLD, Lausanne

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Jacek Dziarmaga

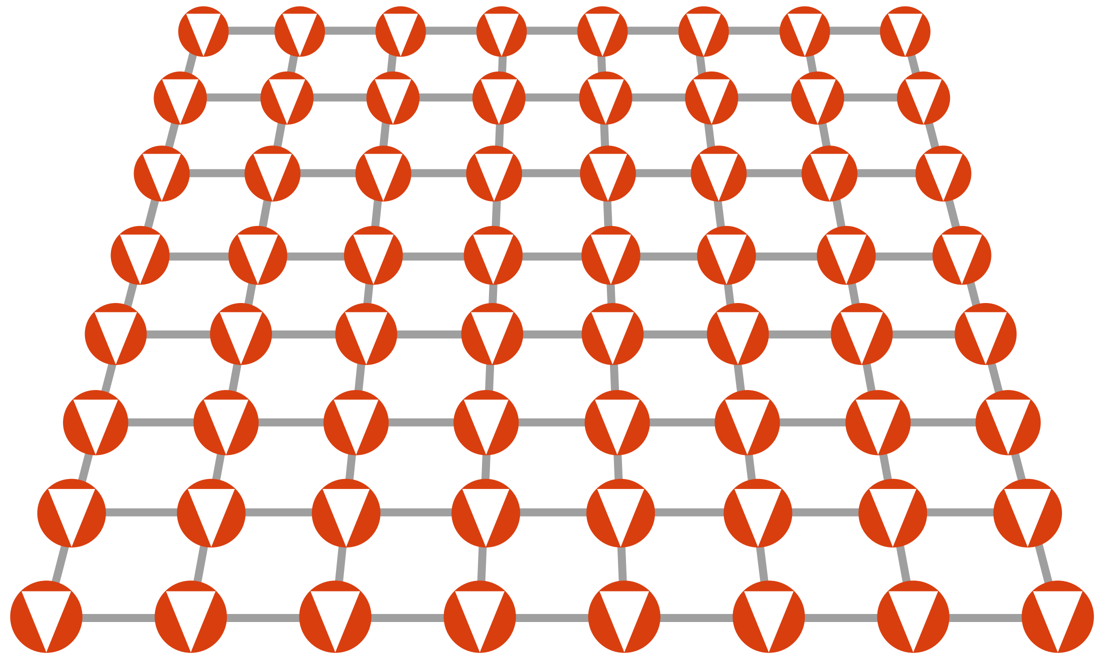
Uni Krakow

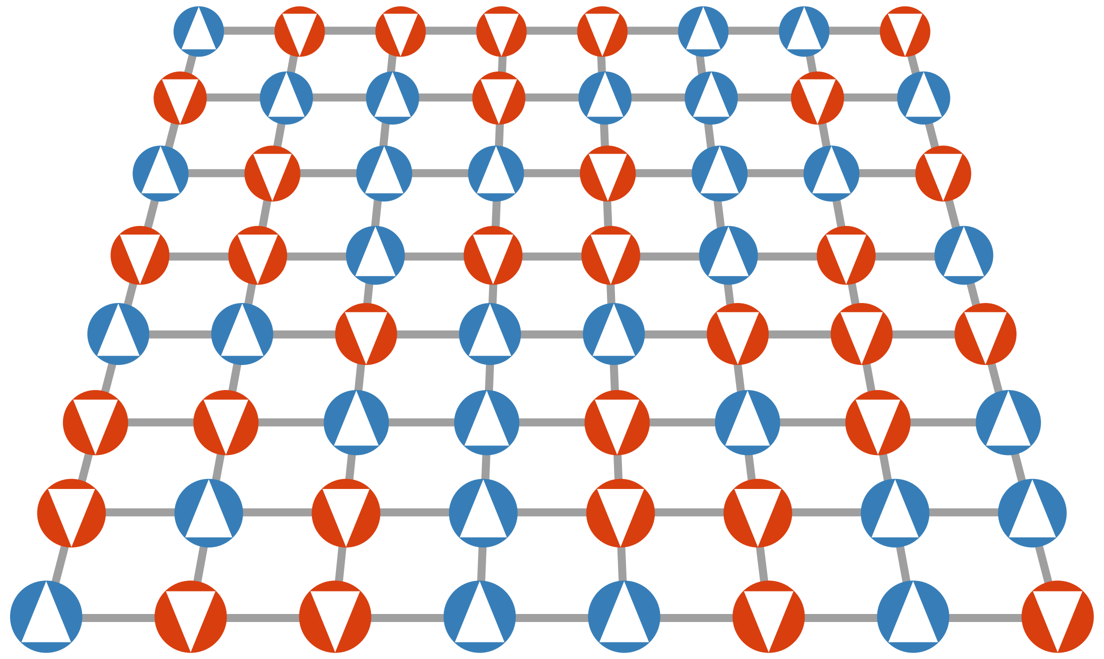
Wojciech Zurek

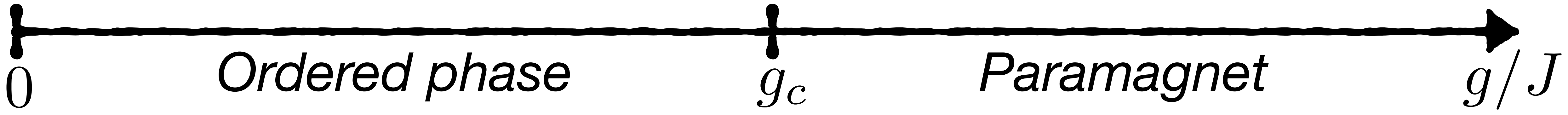
Los Alamos Lab

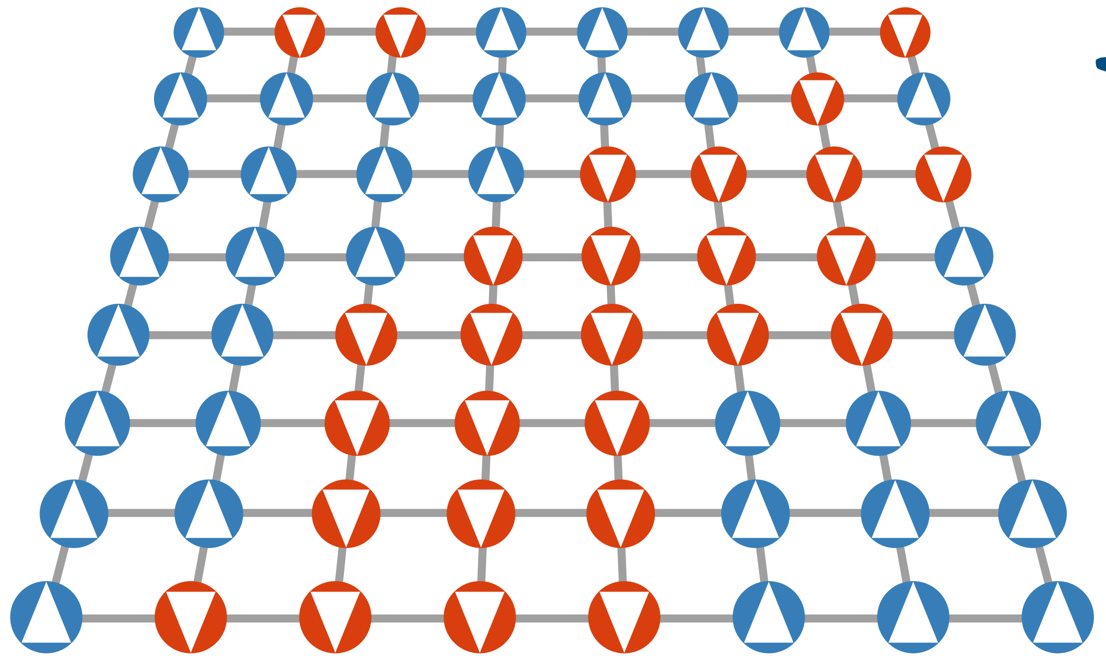
arXiv:2106.09046

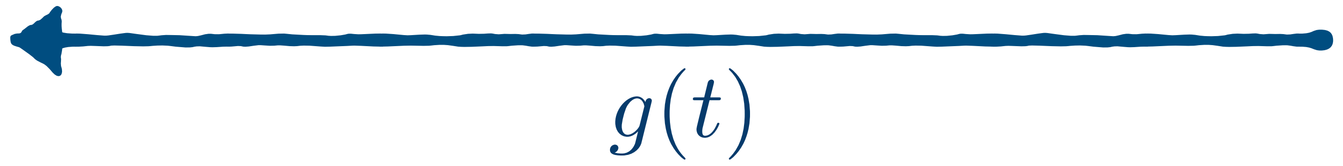
Dynamical universality







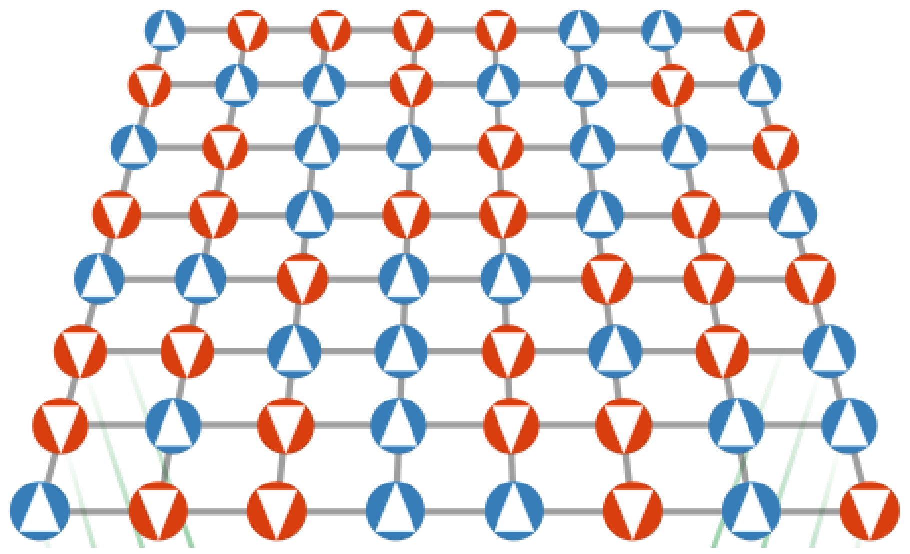




→ **What is the typical size of domains?**

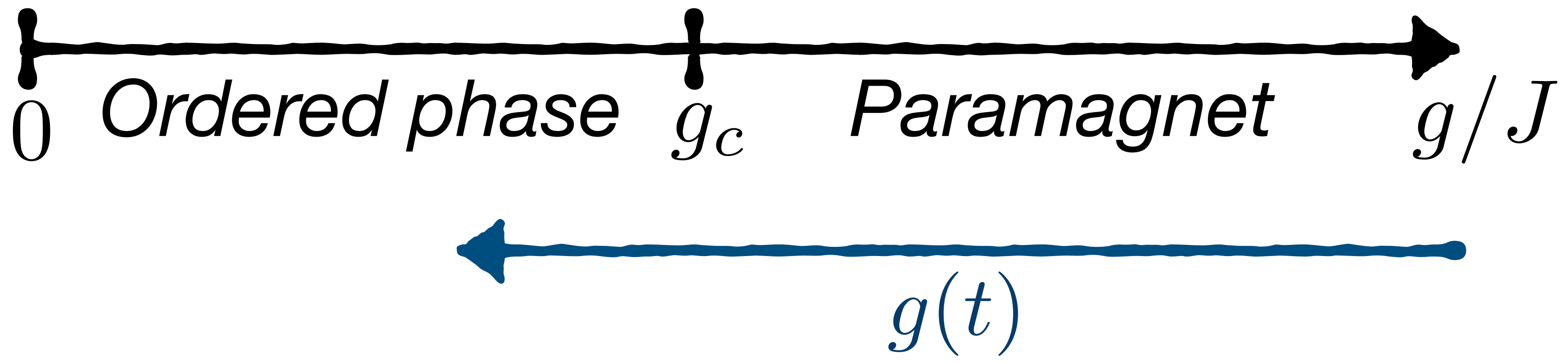
Markus Schmitt, *University of Cologne*

Dynamical universality



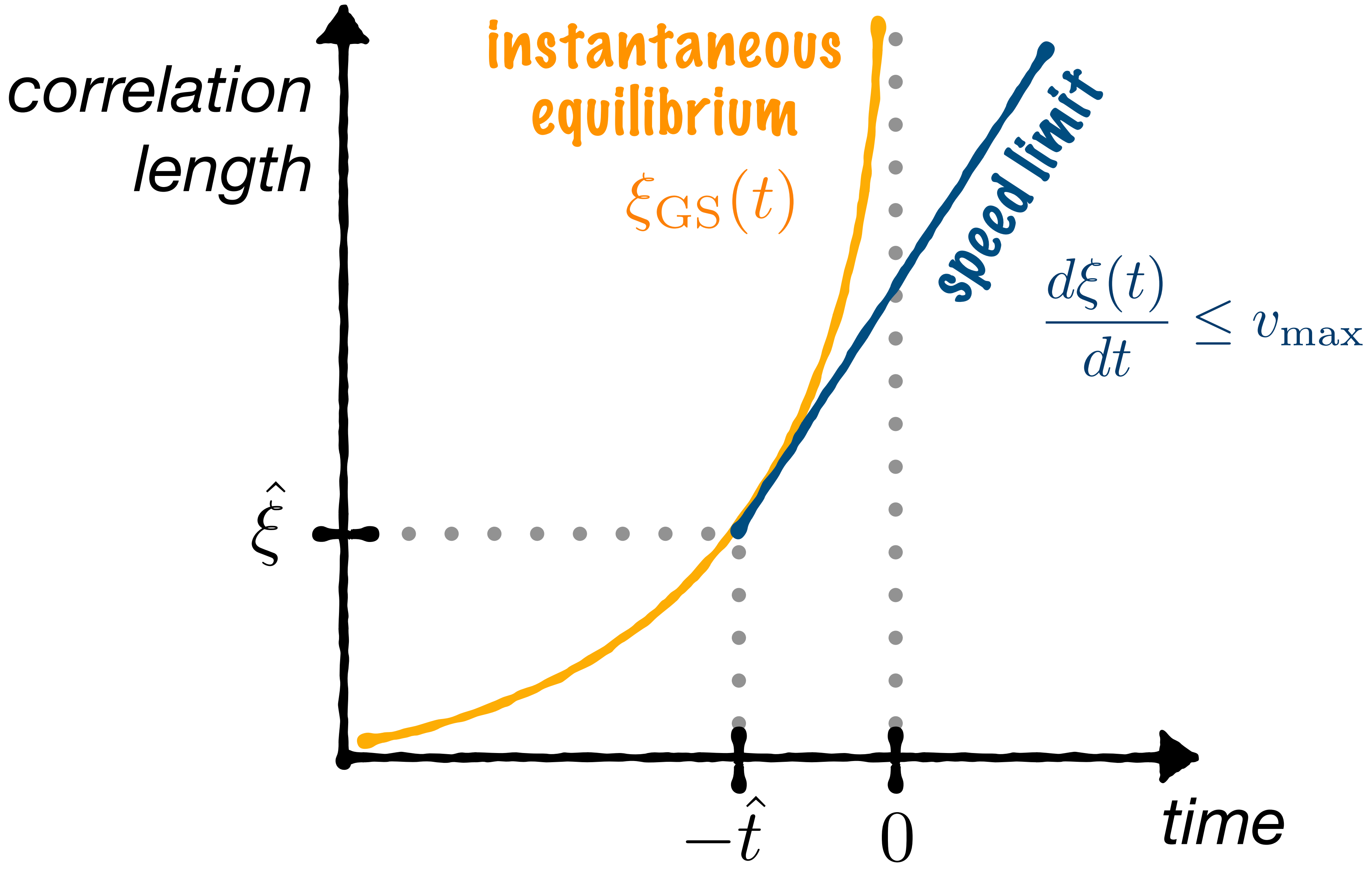
Quantum Ising model

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - g \sum_i \hat{\sigma}_i^x$$



→ **What characterizes excitations** *when the ramp becomes non-adiabatic?*

Kibble, *J. Phys. A: Math. Gen.* (1976)
Zurek, *Nature* (1985)
. . .



Characteristic time and length scales: $\hat{t} \propto \tau_Q^{\frac{z\nu}{1+z\nu}}$ $\quad \hat{\xi} \propto \tau_Q^{\frac{\nu}{1+z\nu}}$

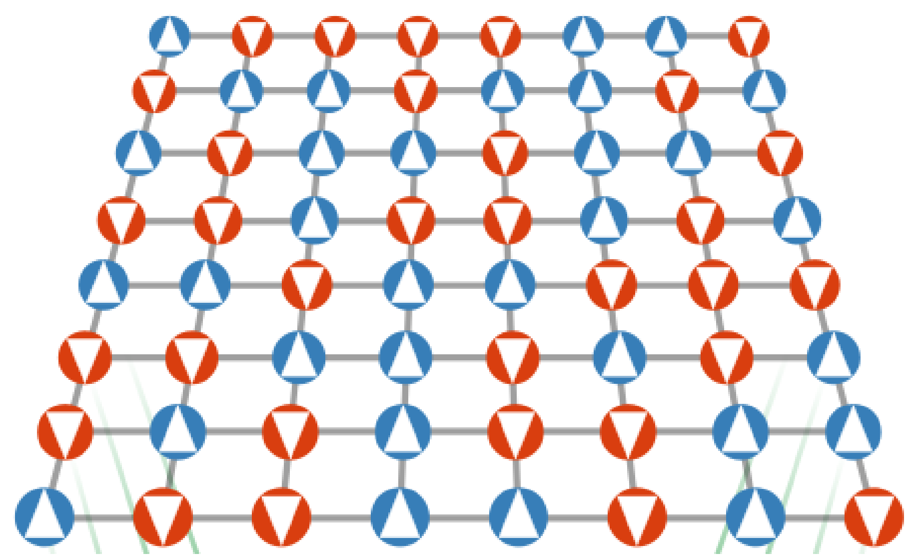
critical exponents

ramping rate

Non-equilibrium scaling hypothesis:

$$O_L(t,R) = \hat{\xi}^{-\Delta_O} F_O(t/\hat{t}, R/\hat{\xi}, \hat{\xi}/L)$$

Quantum simulation: Rydberg atom arrays



Quantum Ising model

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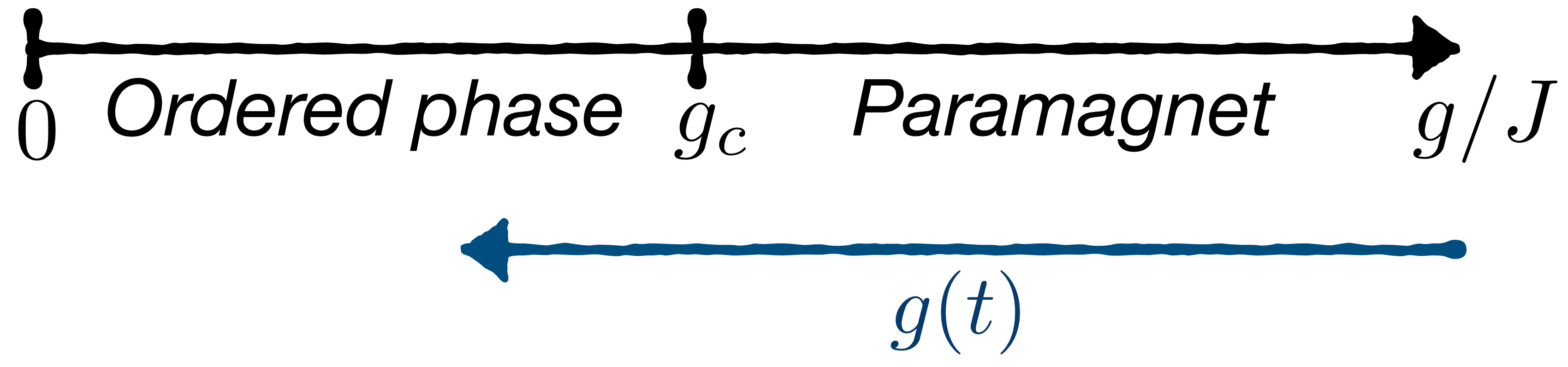
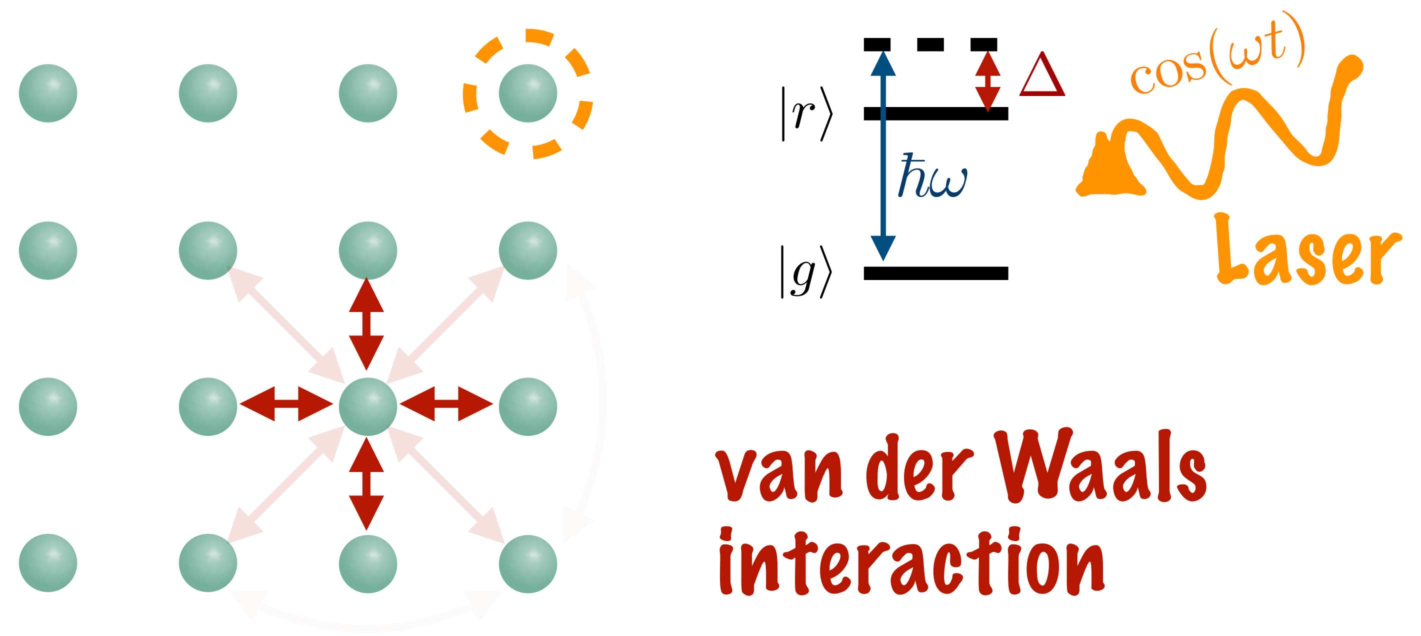
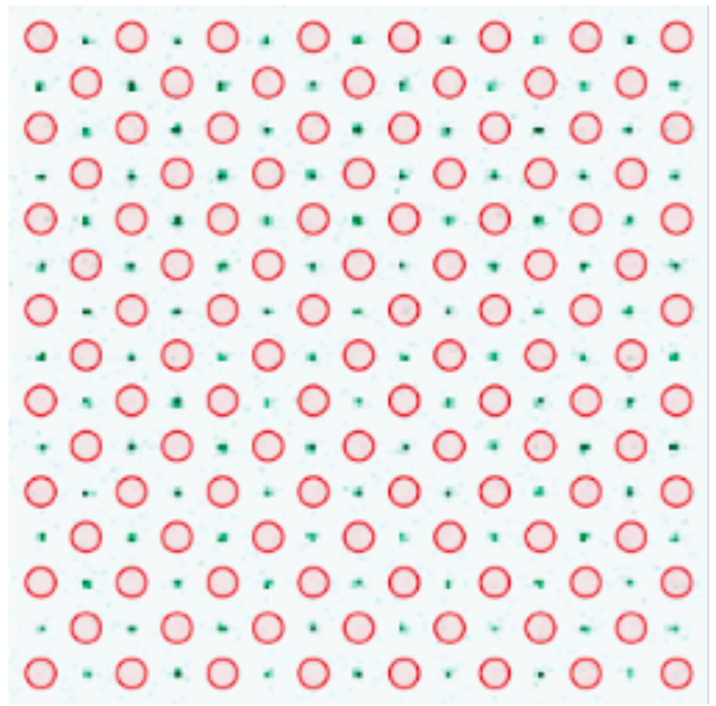


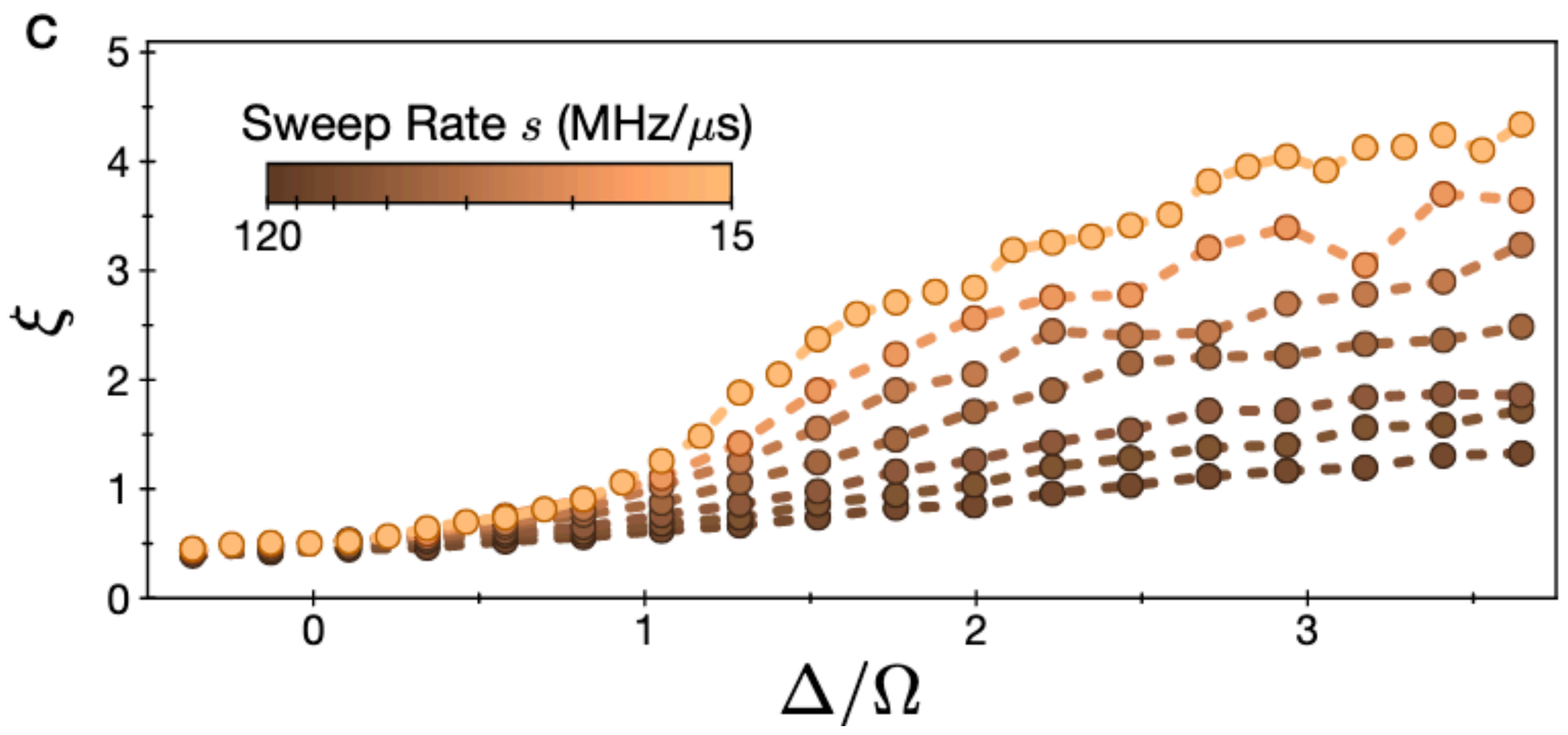
Rydberg atom array



individual atom resolution



time-dependent measurement



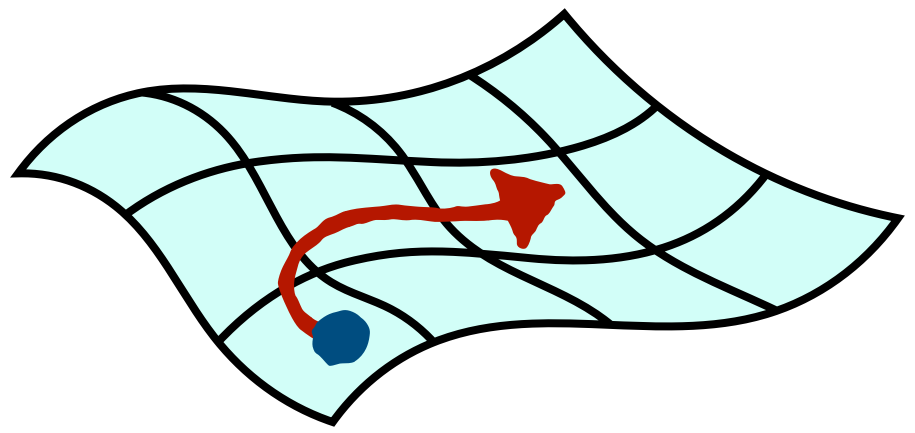
Ebadi *et al.*, Nature 2021

Objective

Simulation of isolated system dynamics ⟷ **Numerical solution of Schrödinger equation**

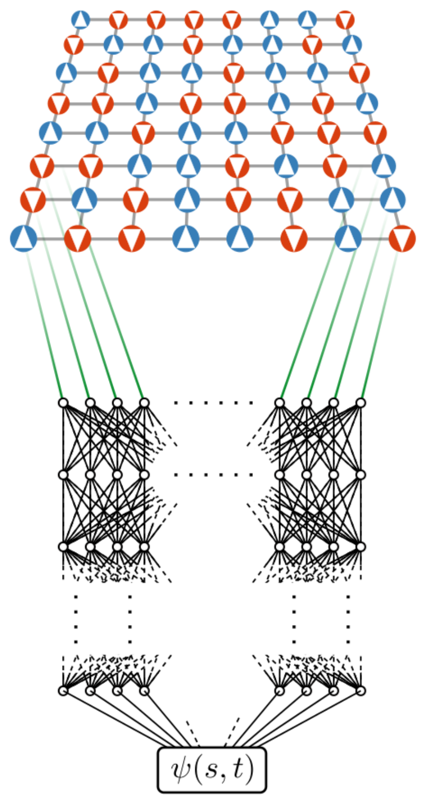
$$i\frac{d}{dt}|\psi\rangle = \hat{H}(t)|\psi\rangle$$

Outline



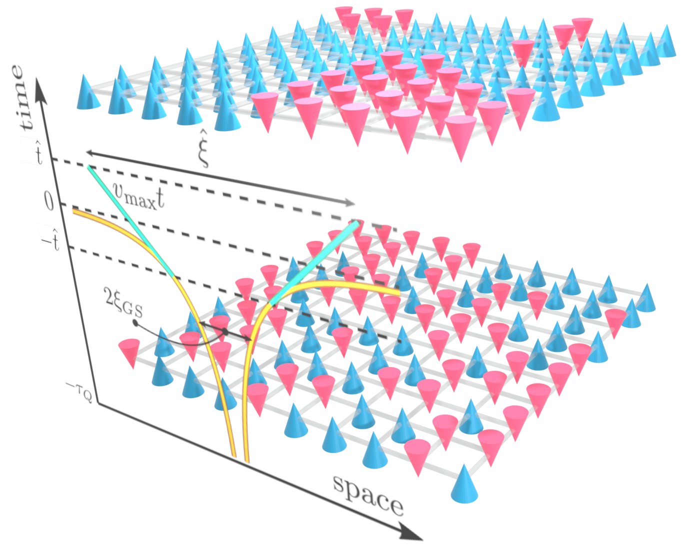
Numerical machinery

Time-dependent variational principle



Deep Learning ingredient

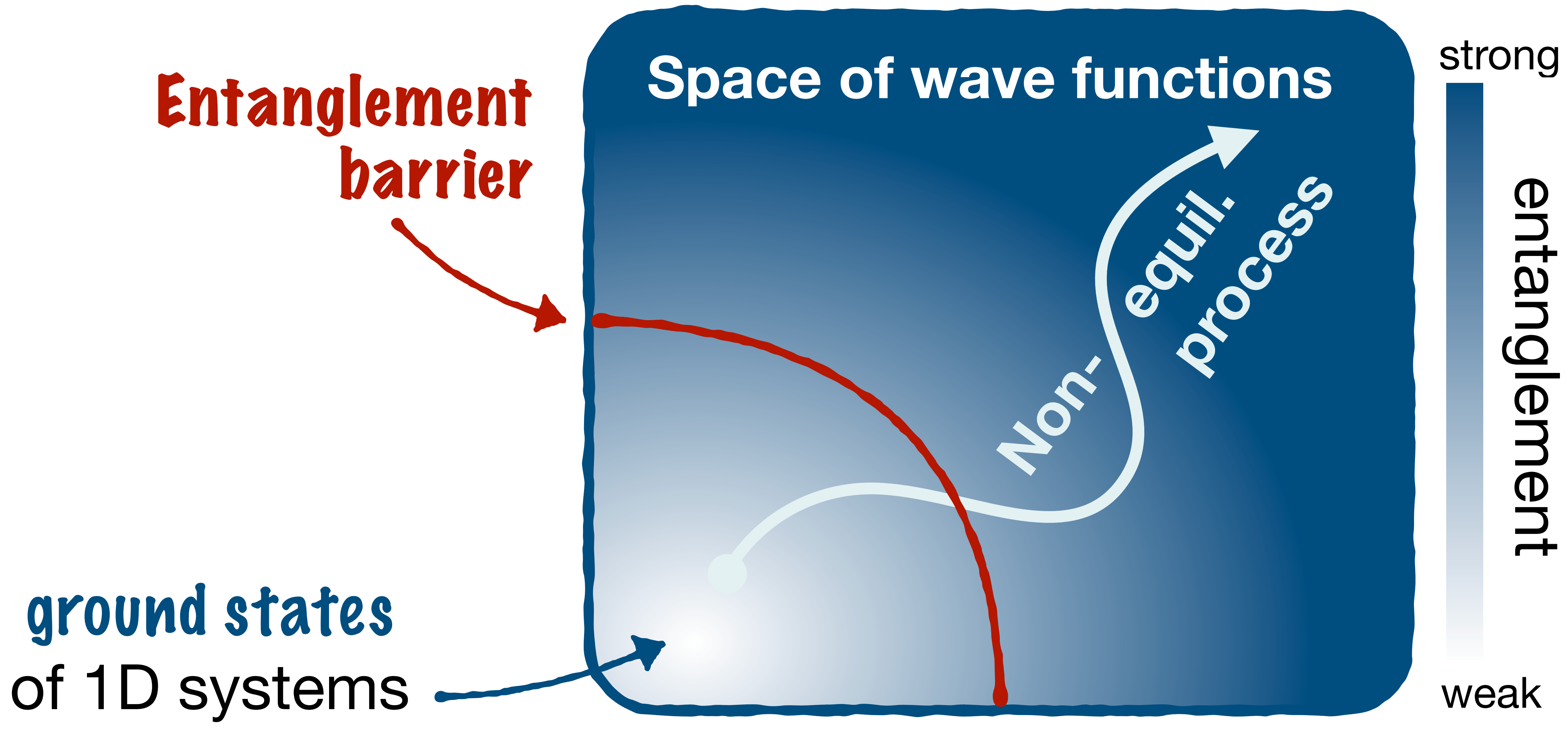
Neural quantum states



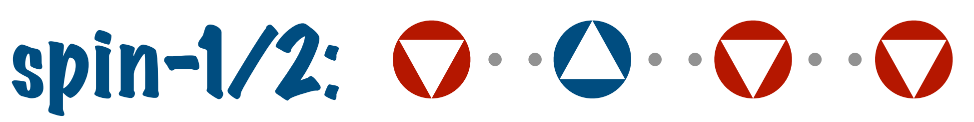
Application

Detecting dynamical universality

Simulations of quantum matter

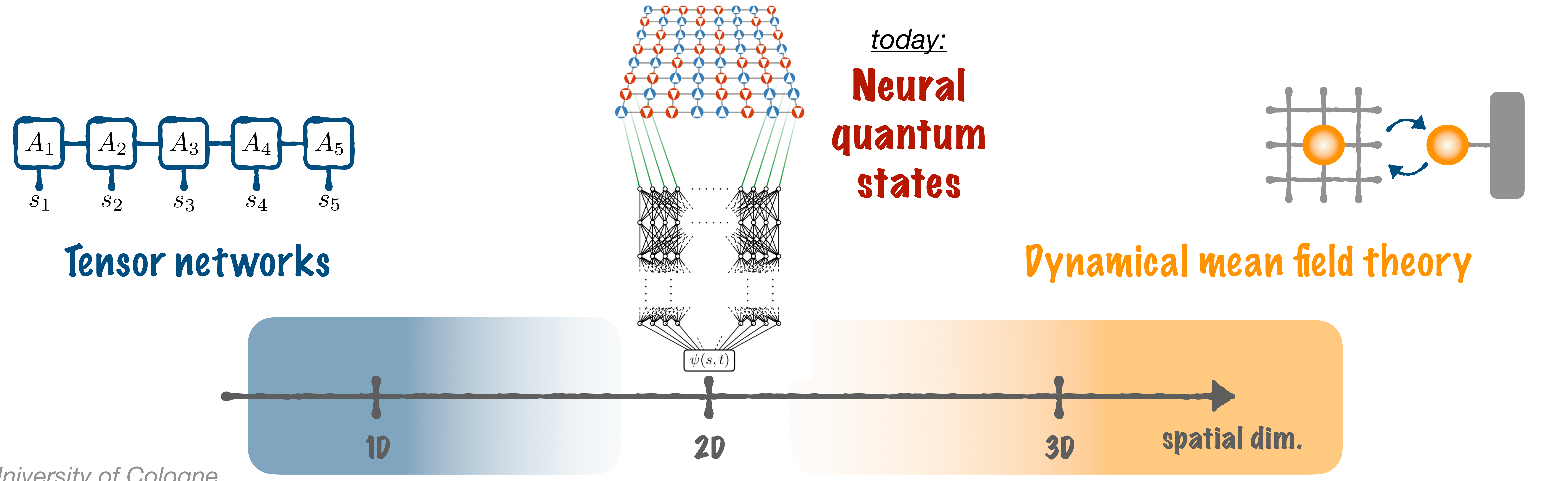


Eisert *et al.*, *Rev. Mod. Phys.* (2010)



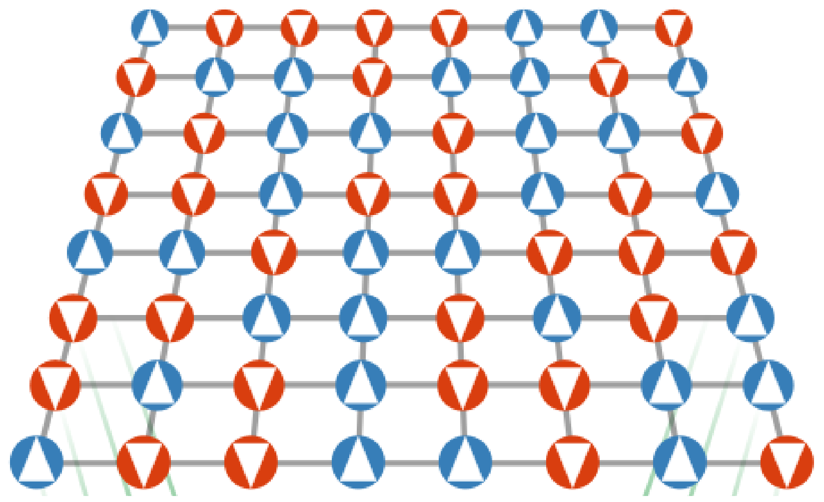
$$|\psi\rangle = \sum_{\mathbf{s}} \psi(\mathbf{s})\, |s_1\rangle \otimes \ldots \otimes |s_N\rangle \quad \in \mathbb{C}^{2^N}$$

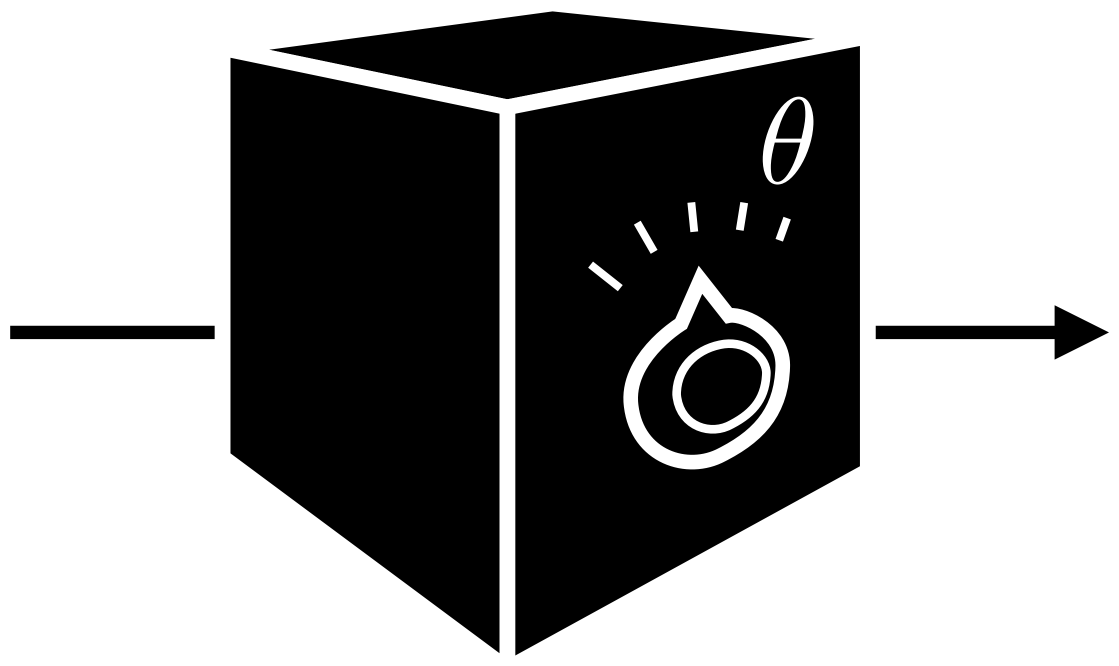
Entanglement **Curse of dimensionality**



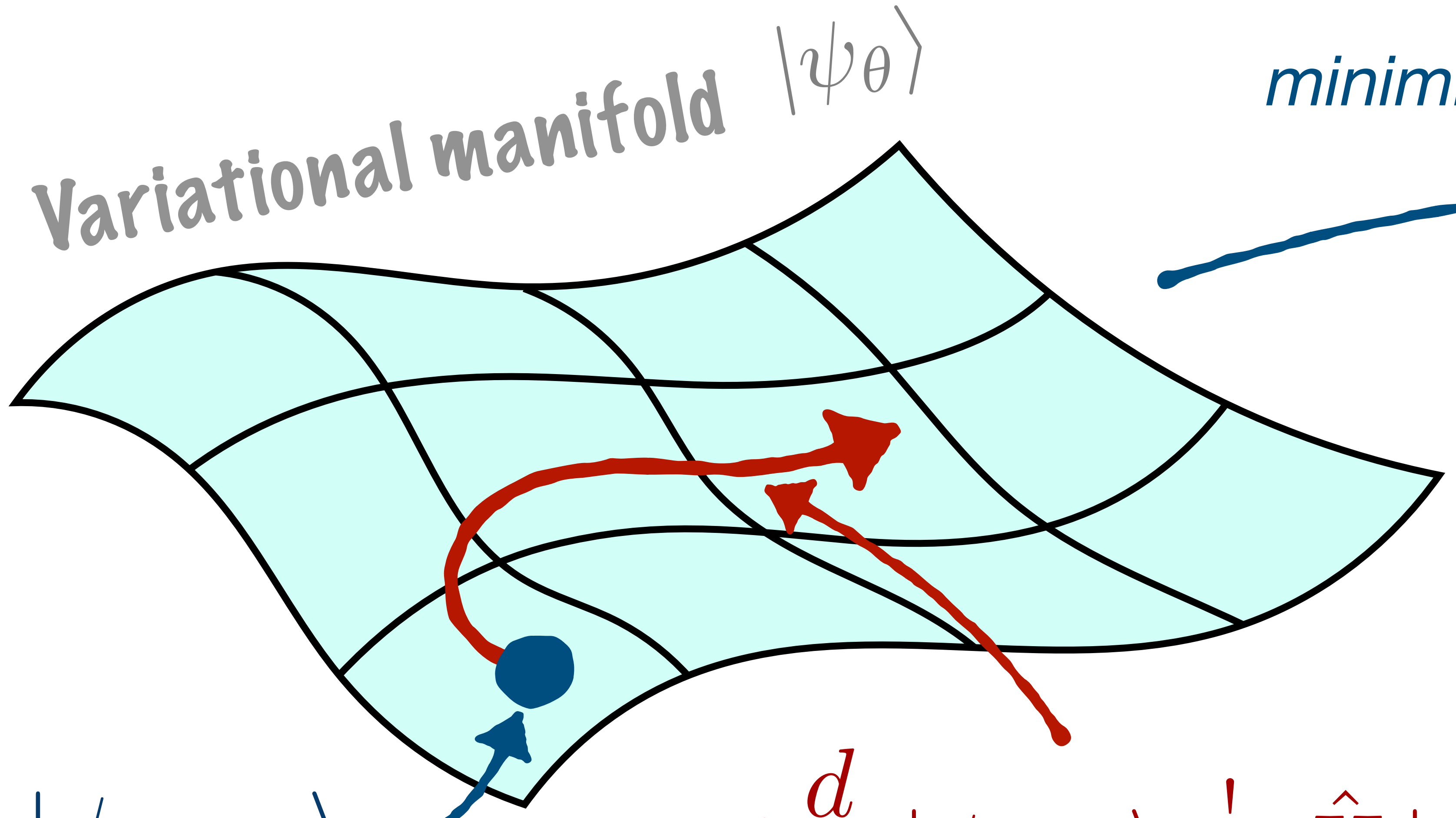
Time-dependent variational principle

$$|\psi_\theta\rangle = \sum_{\mathbf{s}} \psi_\theta(\mathbf{s})\,|\mathbf{s}\rangle$$





$\psi_\theta(\mathbf{s})$



$|\psi_{\theta(t_0)}\rangle$

$$i\frac{d}{dt}|\psi_{\theta(t)}\rangle \stackrel{!}{=} \hat{H}\,|\psi_{\theta(t)}\rangle$$

minimize $\left\| i\frac{d}{dt}|\psi_\theta\rangle - \hat{H}\,|\psi_\theta\rangle \right\|$

Broeckhove *et al.*, *Chem. Phys. Lett.* (1988)

$$S_{k,k'}\dot{\theta}_{k'} = -iF_k$$

Hamiltonian $\hat{H}$

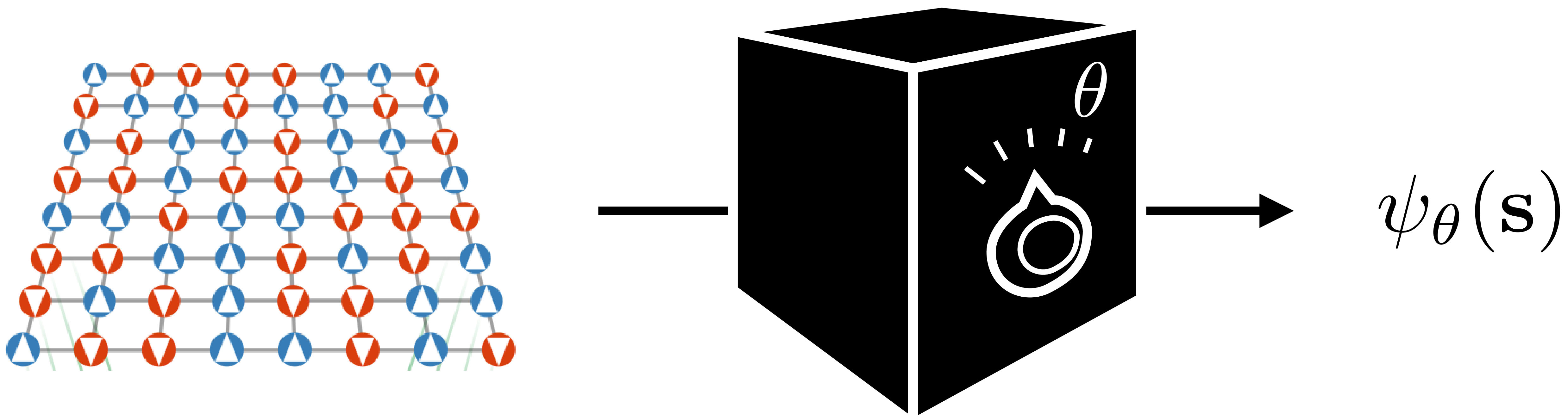
Quantum metric tensor

driving “force”

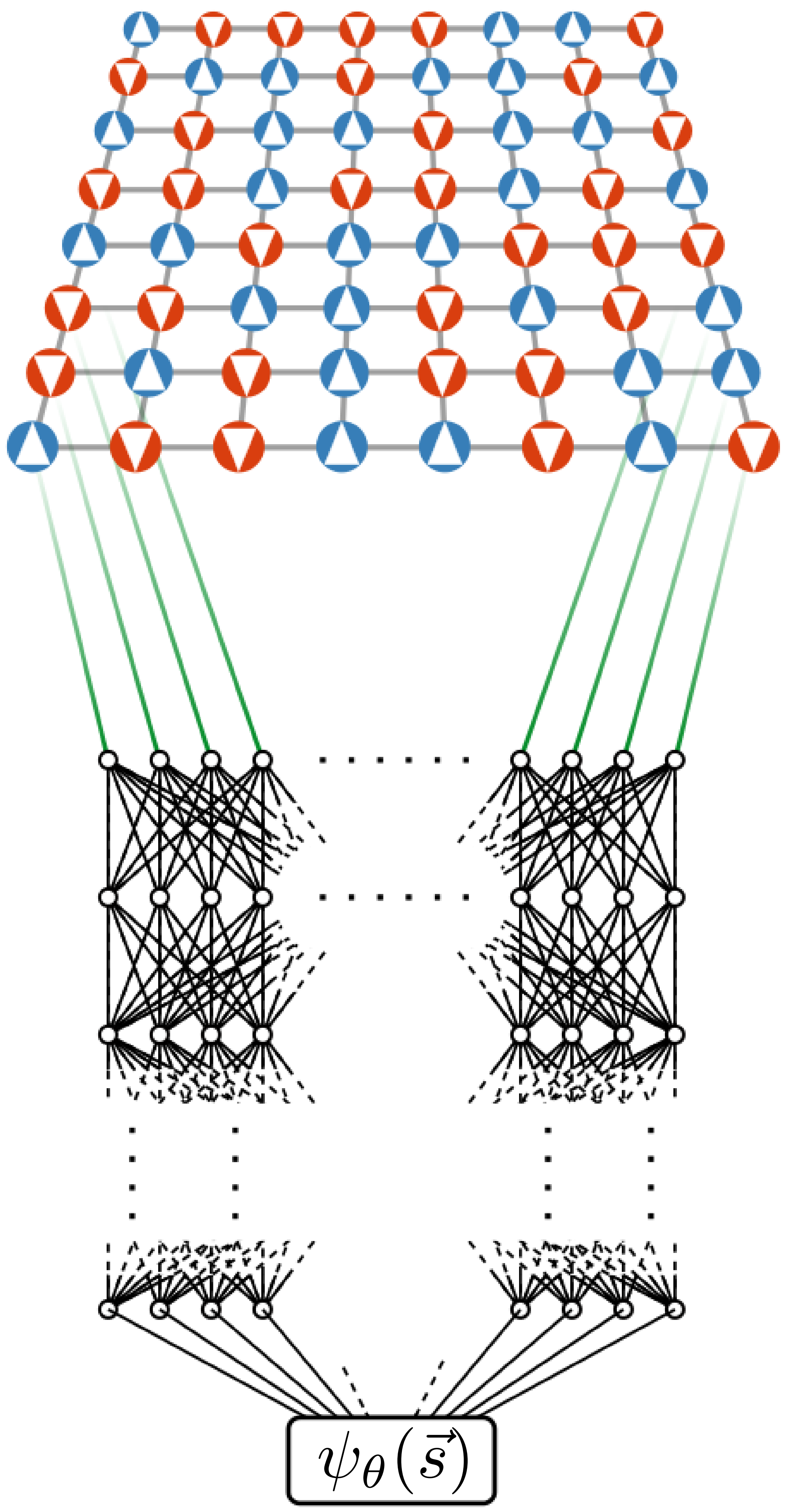
$$S_{k,k'} = \langle \partial_{\theta_k}\psi_\theta | \partial_{\theta_{k'}}\psi_\theta\rangle_c$$

$$F_k = \langle \partial_{\theta_k}\psi_\theta | \hat{H} | \psi_\theta\rangle_c$$

Neural quantum states



Neural Quantum States



Proposed by Carleo and Troyer, *Science* (2017)

→ **Universal function approximator**

A. N. Kolmogorov, *Dokl. Akad. Nauk SSSR* (1961)
K. Hornik, *Neural Netw.* (1991)

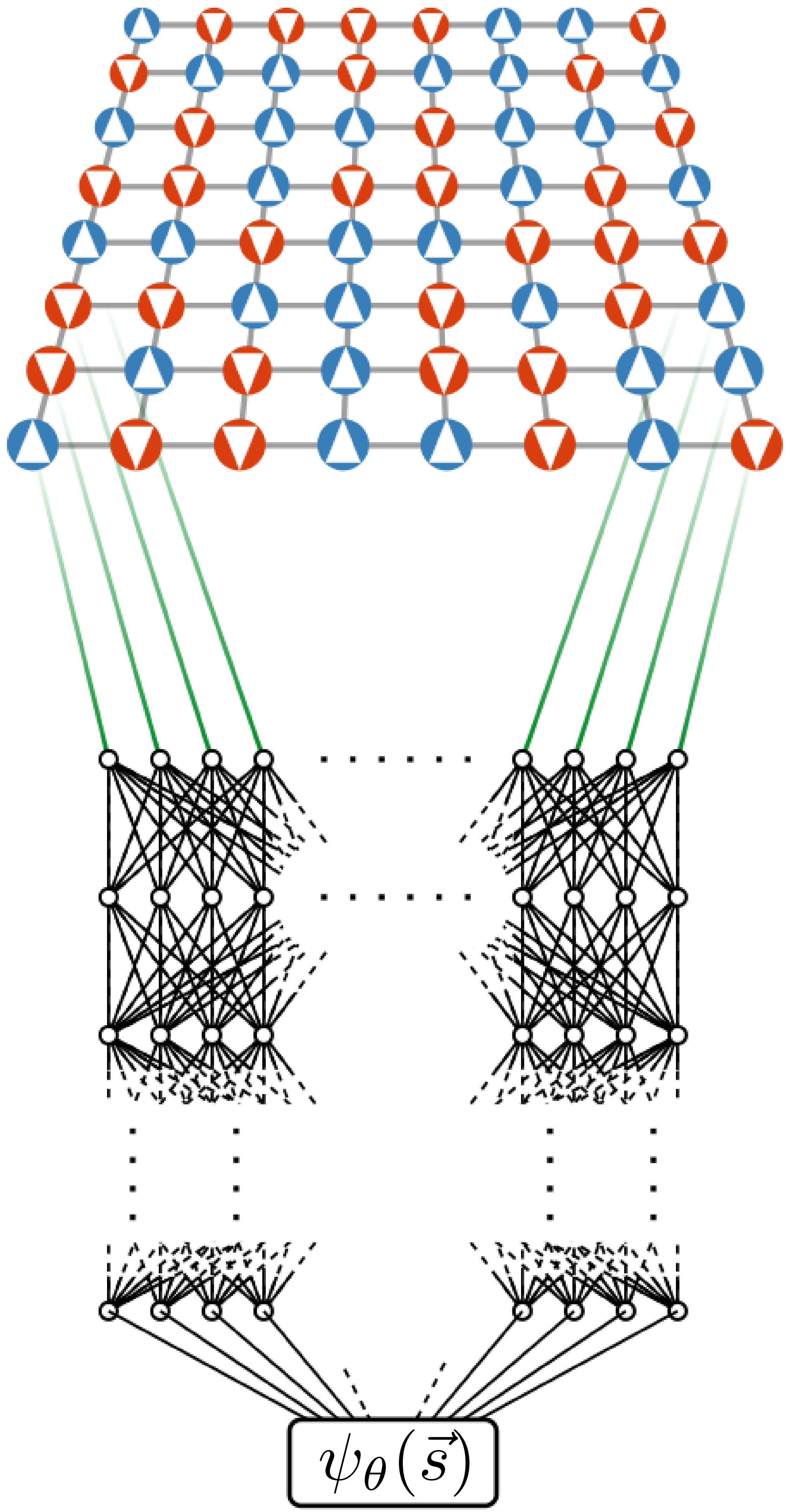
network size = control parameter

→ *numerically exact approach*

→ Exploitation of **large scale computing** resources

(multi-node GPU clusters)

Neural Quantum States



Design principles

→ **Symmetries**

Build in invariance under physical symmetries

example: Convolutional neural networks

Carleo and Troyer, *Science* (2017)
Choo *et al.*, *Phys. Rev. Lett.* (2018)
Vieijra *et al.*, *Phys. Rev. Lett.* (2020)
...

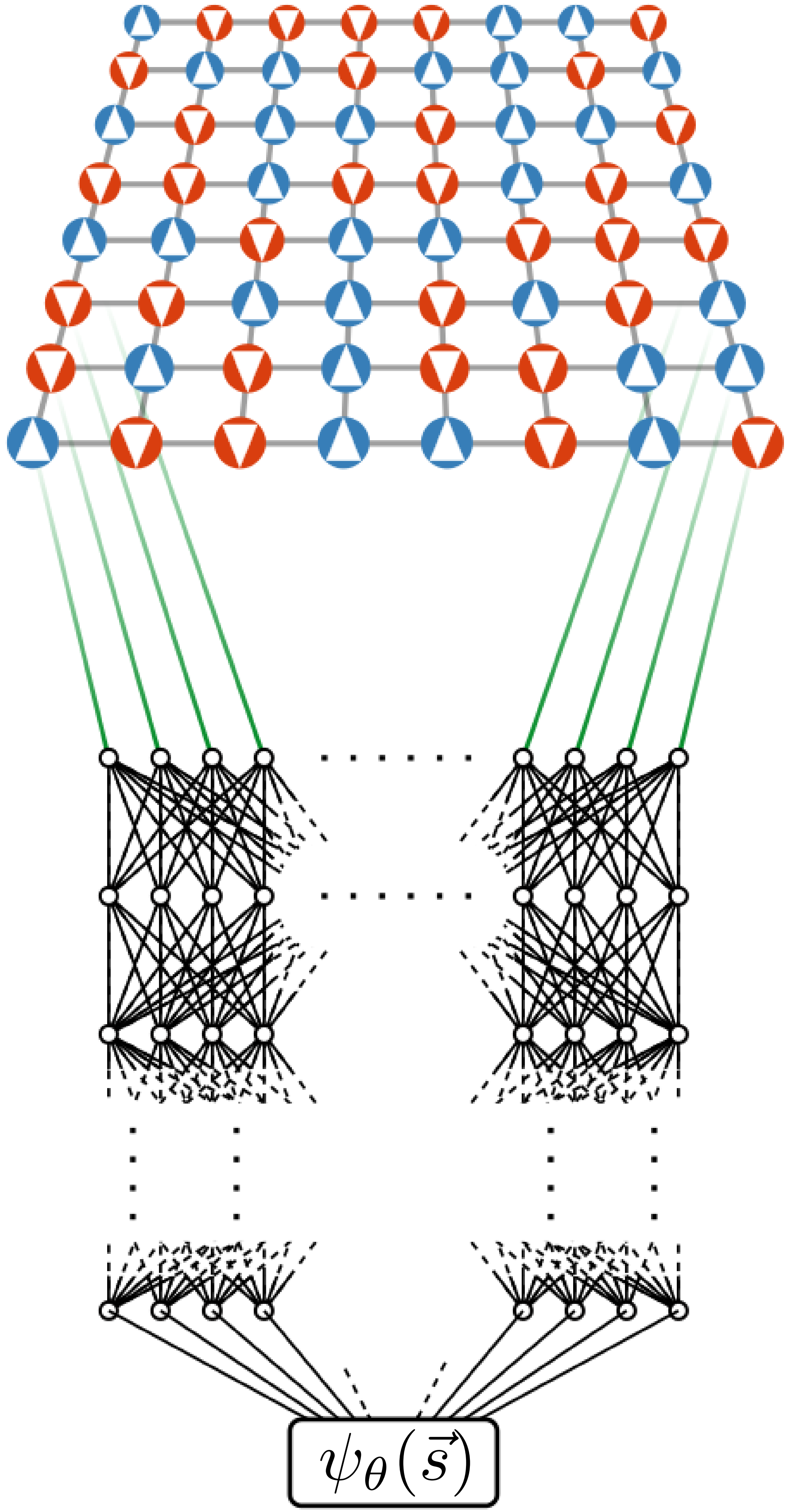
→ **Autoregressive property**

Inherent normalization and direct sampling

example: Recurrent neural networks

Sharir *et al.*, *Phys. Rev. Lett.* (2020)
Hibat-Allah *et al.*, *PRR* (2020)
Reh, Schmitt, and Gärttner, *Phys. Rev. Lett.* (2021)
...

Behind the scenes



+

time-dependent

severely **ill-conditioned**

computed by **sampling of** $|\psi_\theta(\mathbf{s})|^2$ *

$$S_{k,k'}\dot{\theta}_{k'} = -iF_k$$

=

$$^{*}\langle\partial_{\theta_k}\psi_\theta|\hat{H}|\psi_\theta\rangle = \sum_{\mathbf{s}} |\psi_\theta(\mathbf{s})|^2 \left(\partial_{\theta_k} \log\psi_\theta(\mathbf{s}) \frac{\langle\mathbf{s}|\hat{H}|\psi_\theta\rangle}{\psi_\theta(\mathbf{s})}\right)$$

probability

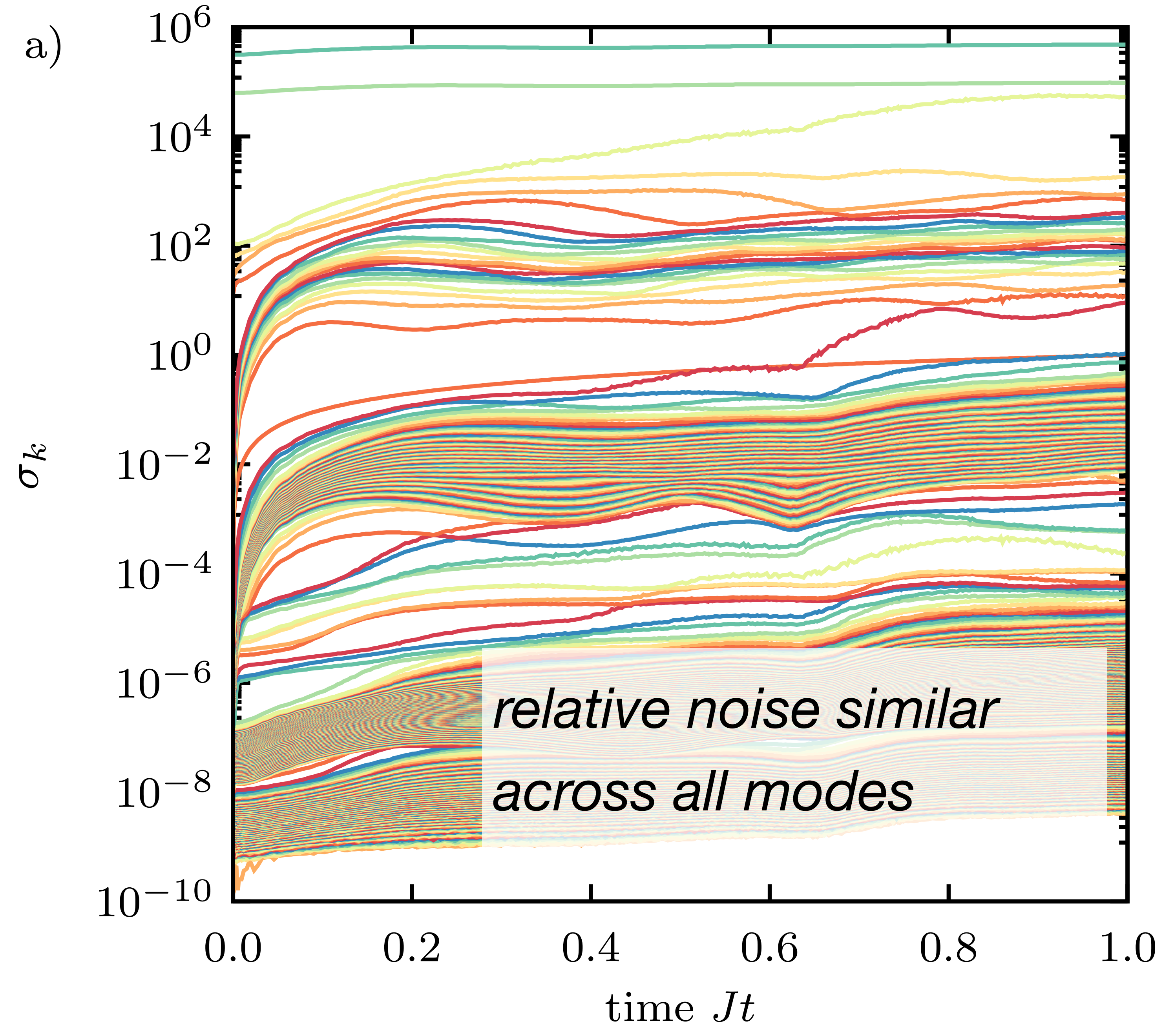
Behind the scenes: Noisy TDVP

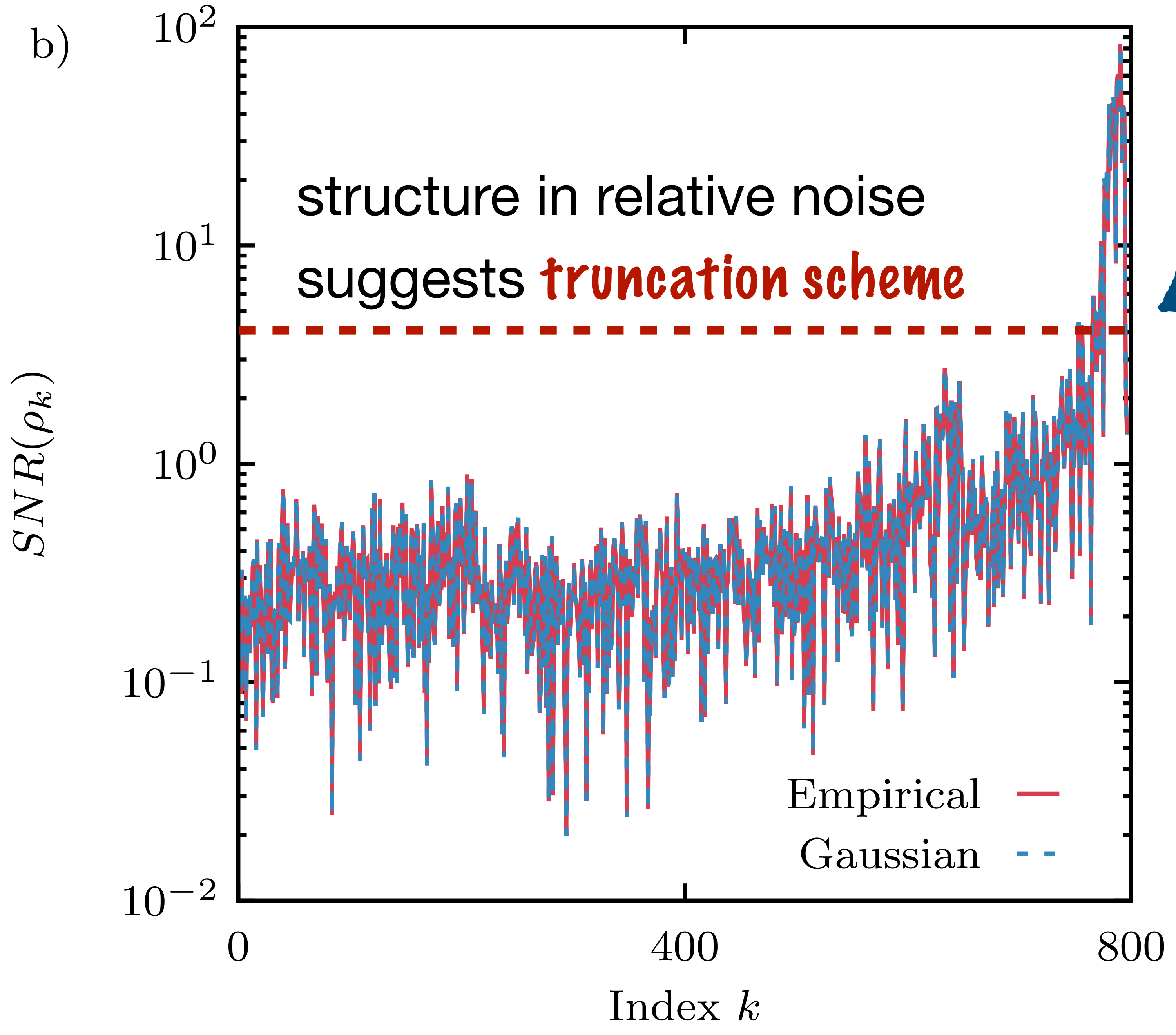
Schmitt and Heyl, *Phys. Rev. Lett.* (2020)

$$S_{k,k'}\dot{\theta}_{k'} = -iF_k$$

in eigenbasis

Specifically eliminate noisy contributions





Remark:

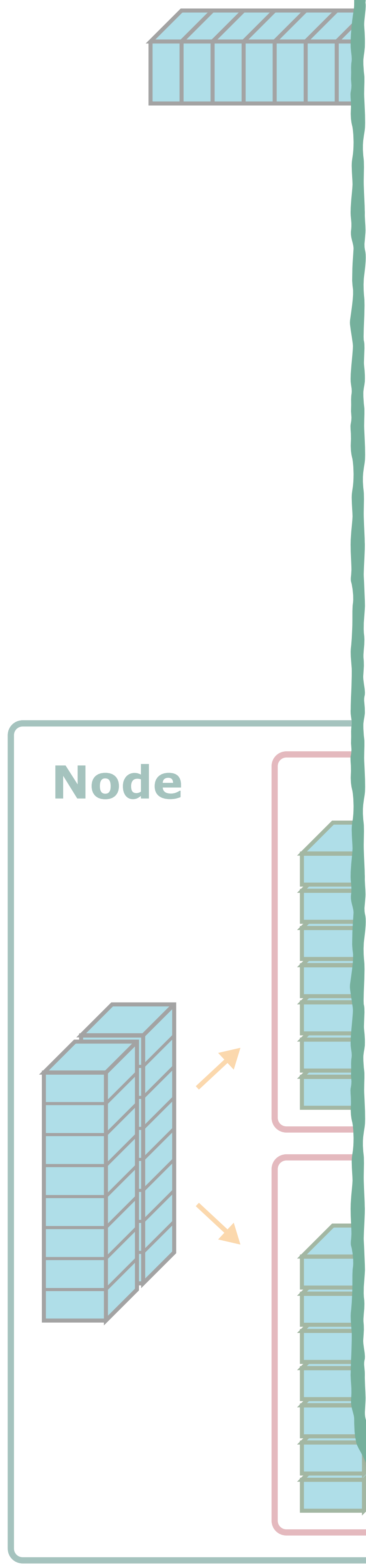
Gradients O_k Gaussian

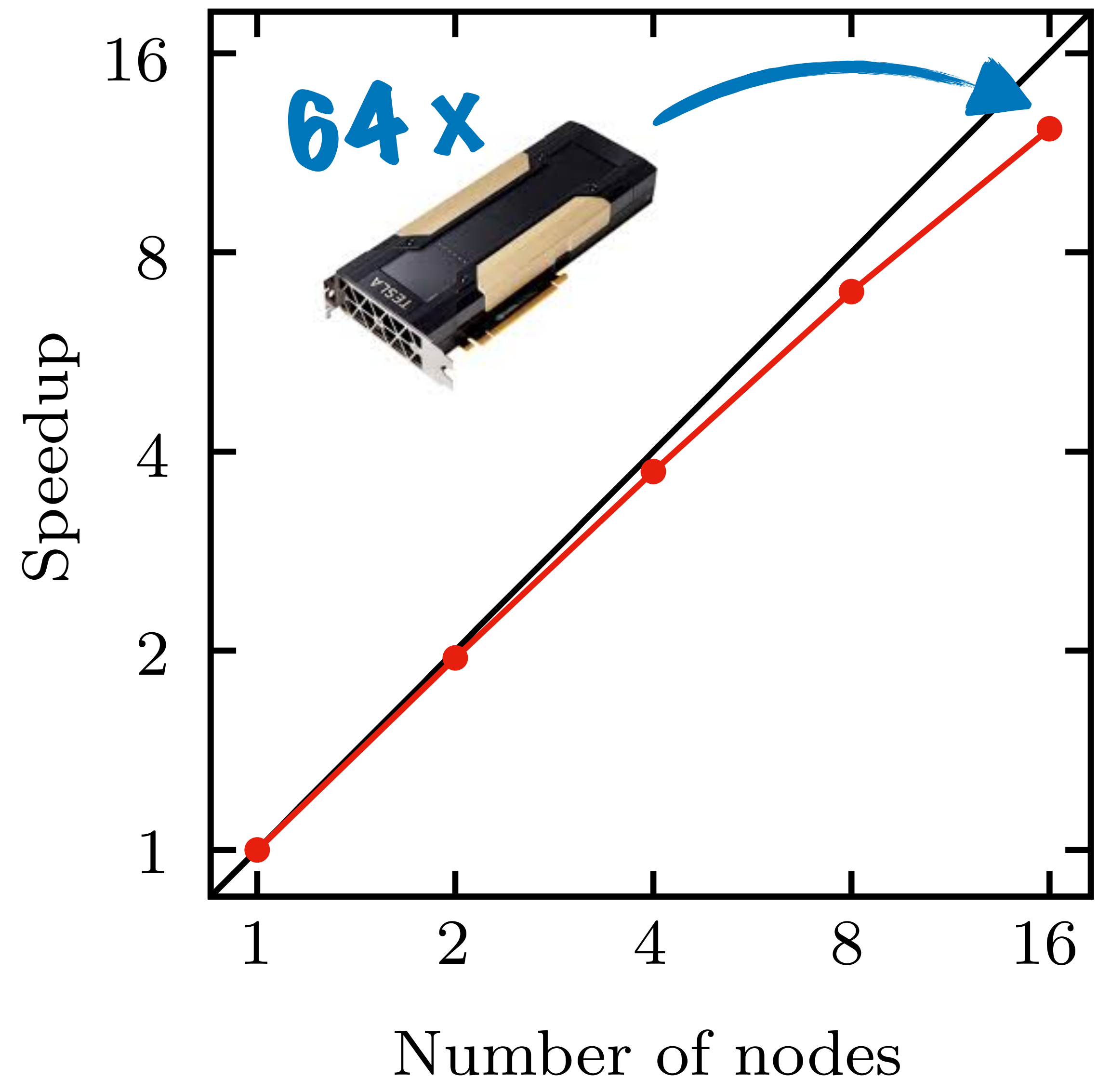
$\Downarrow$

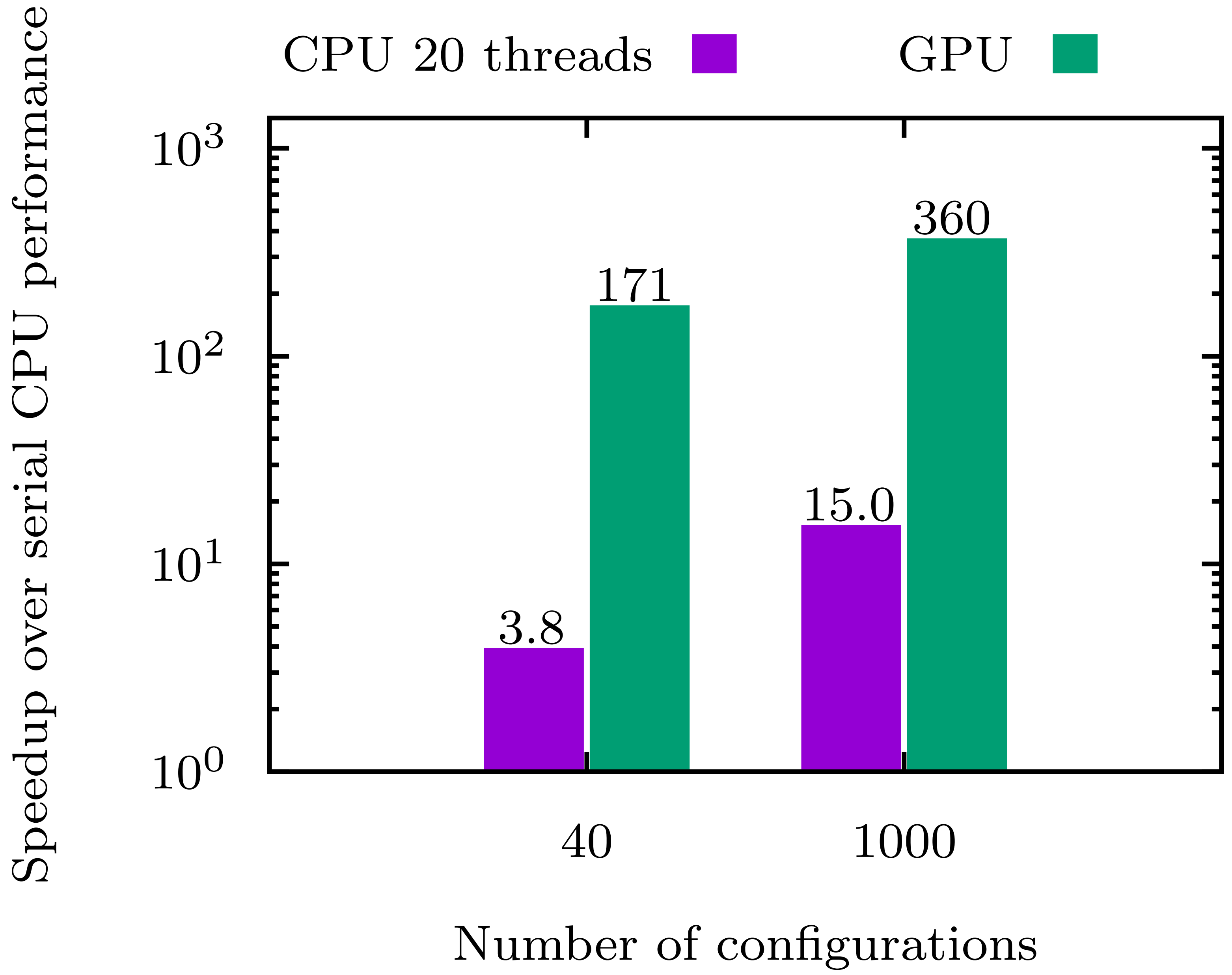
large SNR $\Leftrightarrow$ *High significance for TDVP*

Behind the scenes: Parallelization

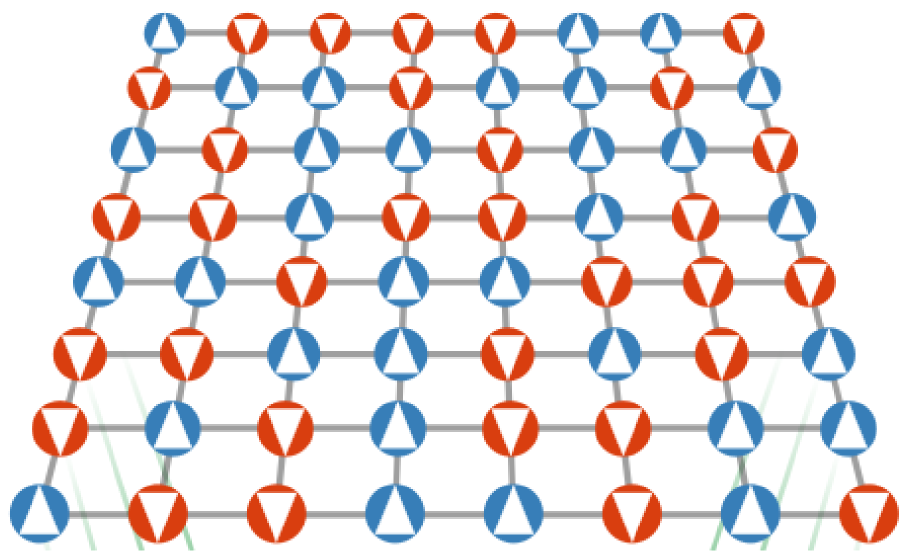
Schmitt and Reh, *arXiv:2108.03409*







Results



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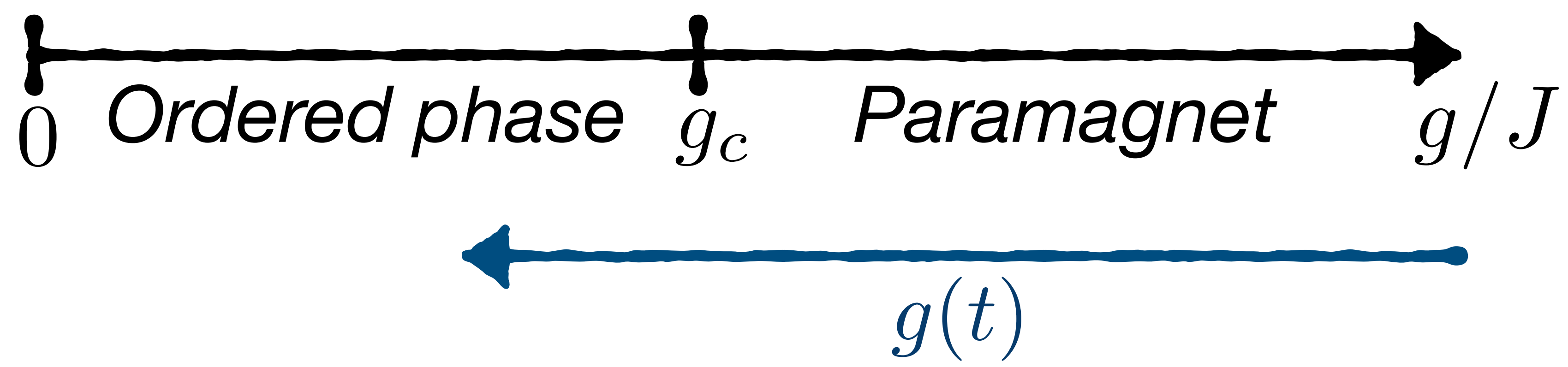
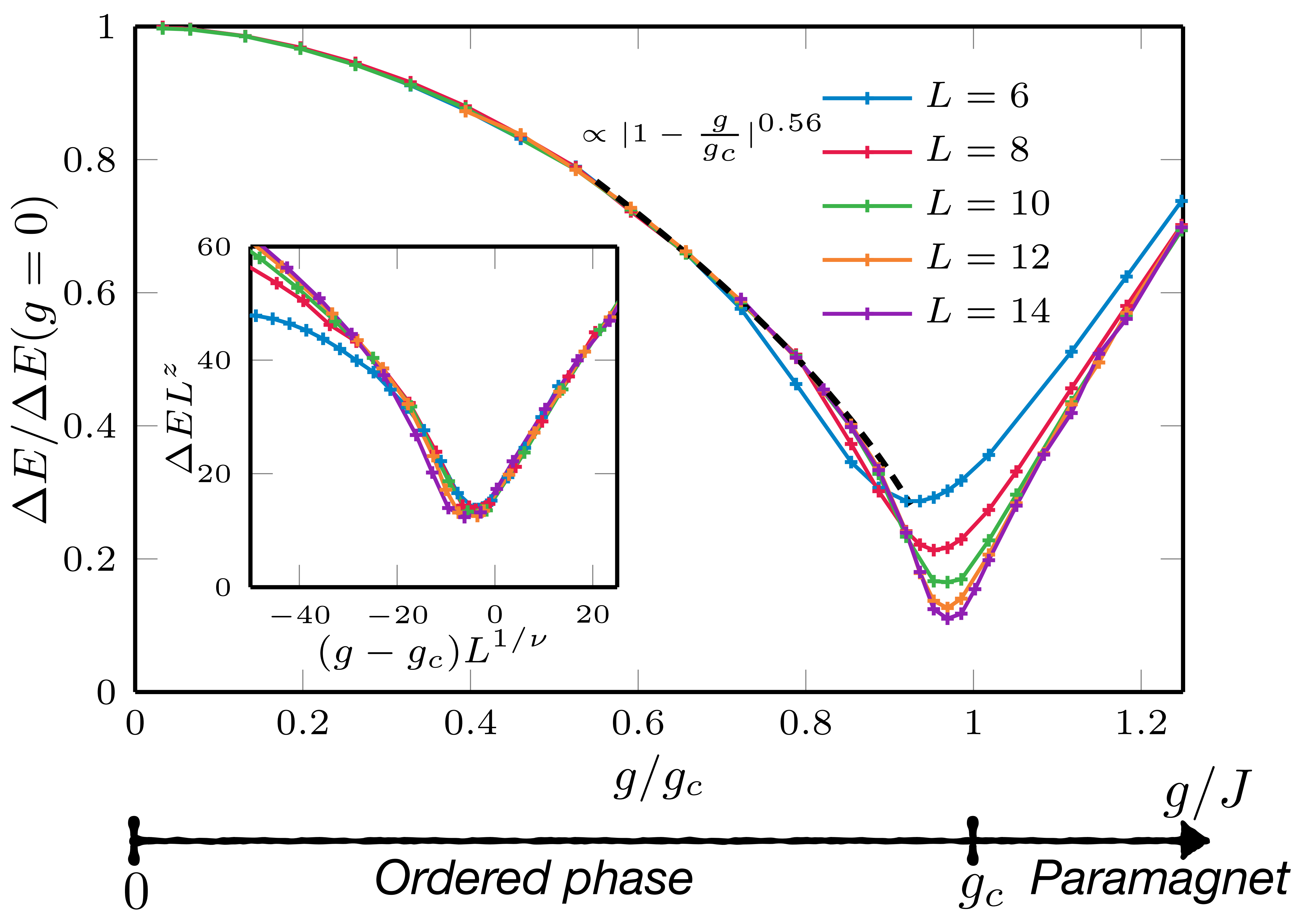


Energy gap

Schmitt, Rams, Dziarmaga, Heyl, and Zurek, *arXiv:2106.09046*



Energy gap between lowest and first excited state

Generally: $\Delta E \propto |g-g_c|^{z\nu}$

Critical exponents known: $z=1\ ,\quad \nu\approx 0.63$

Here: $\Delta E_{\text{fit}} \approx 9.6(4)(g_c\epsilon)^{0.56(3)}$

$(z\nu)_{\text{fit}}$

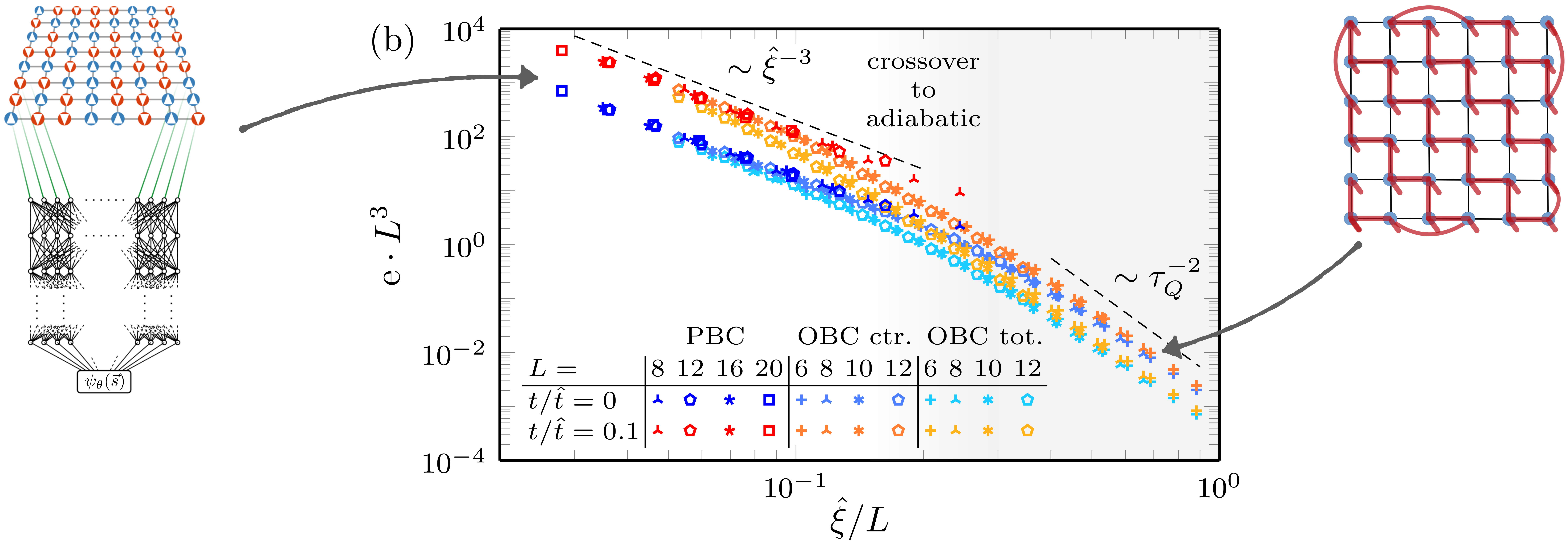
Excited state search Choo *et al.*, *Phys. Rev. Lett.* (2018)

1) *Find ground state* $|\Psi_0\rangle$
2) *Find lowest energy state orthogonal to* $|\Psi_0\rangle$

Excitation energy density

Schmitt, Rams, Dziarmaga, Heyl, and Zurek, *arXiv:2106.09046*

$$\mathrm{e} = \frac{1}{L^2}\left(\langle H(t)\rangle - E_0(t)\right)$$



Perfect collapse in the vicinity of the critical point with known scaling dimensions and $(z\nu)_{\mathrm{fit}}$

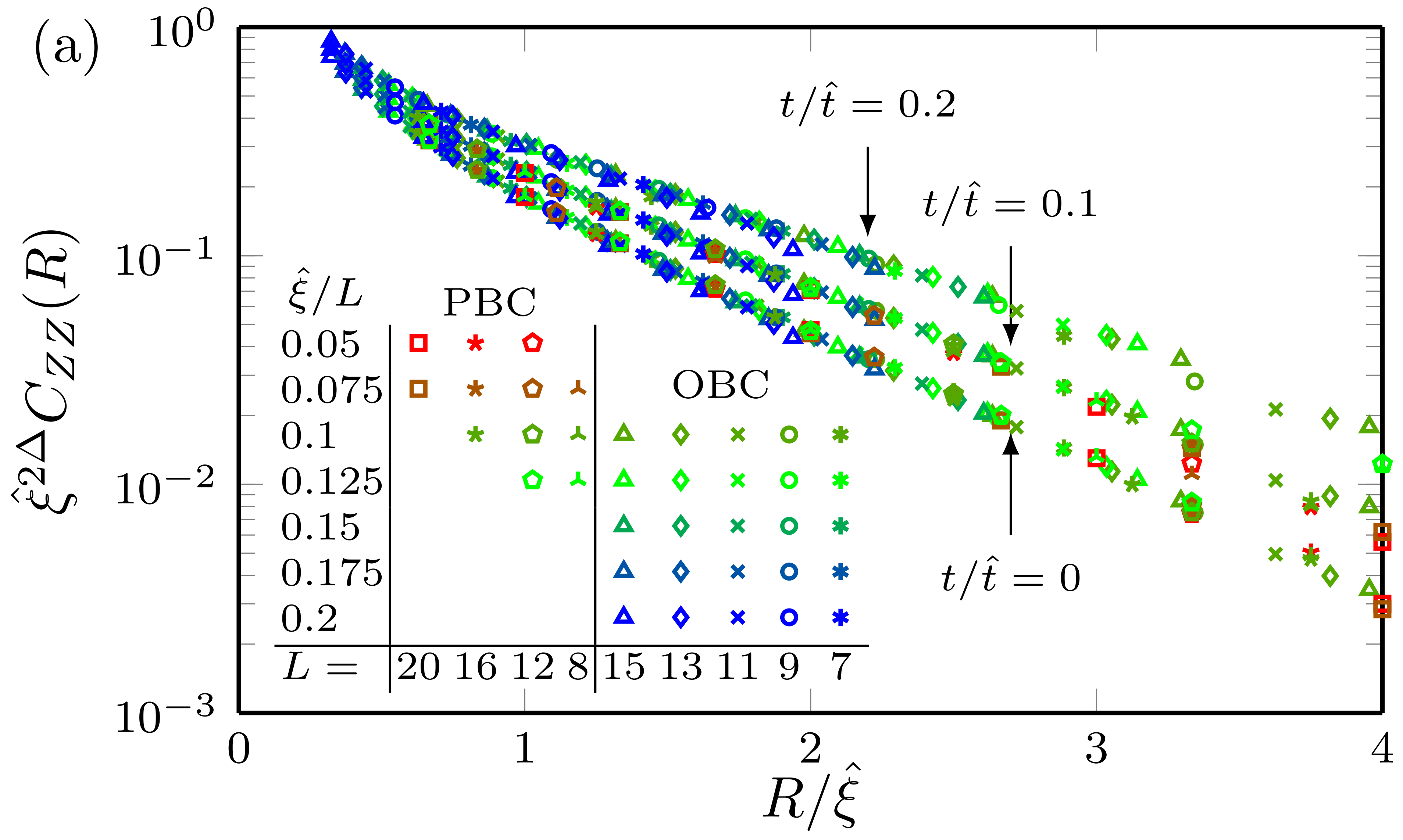
— despite rather small system sizes

Correlation function

Numerical simulation with NQS and Tensor Networks

Schmitt, Rams, Dziarmaga, Heyl, and Zurek, *arXiv:2106.09046*

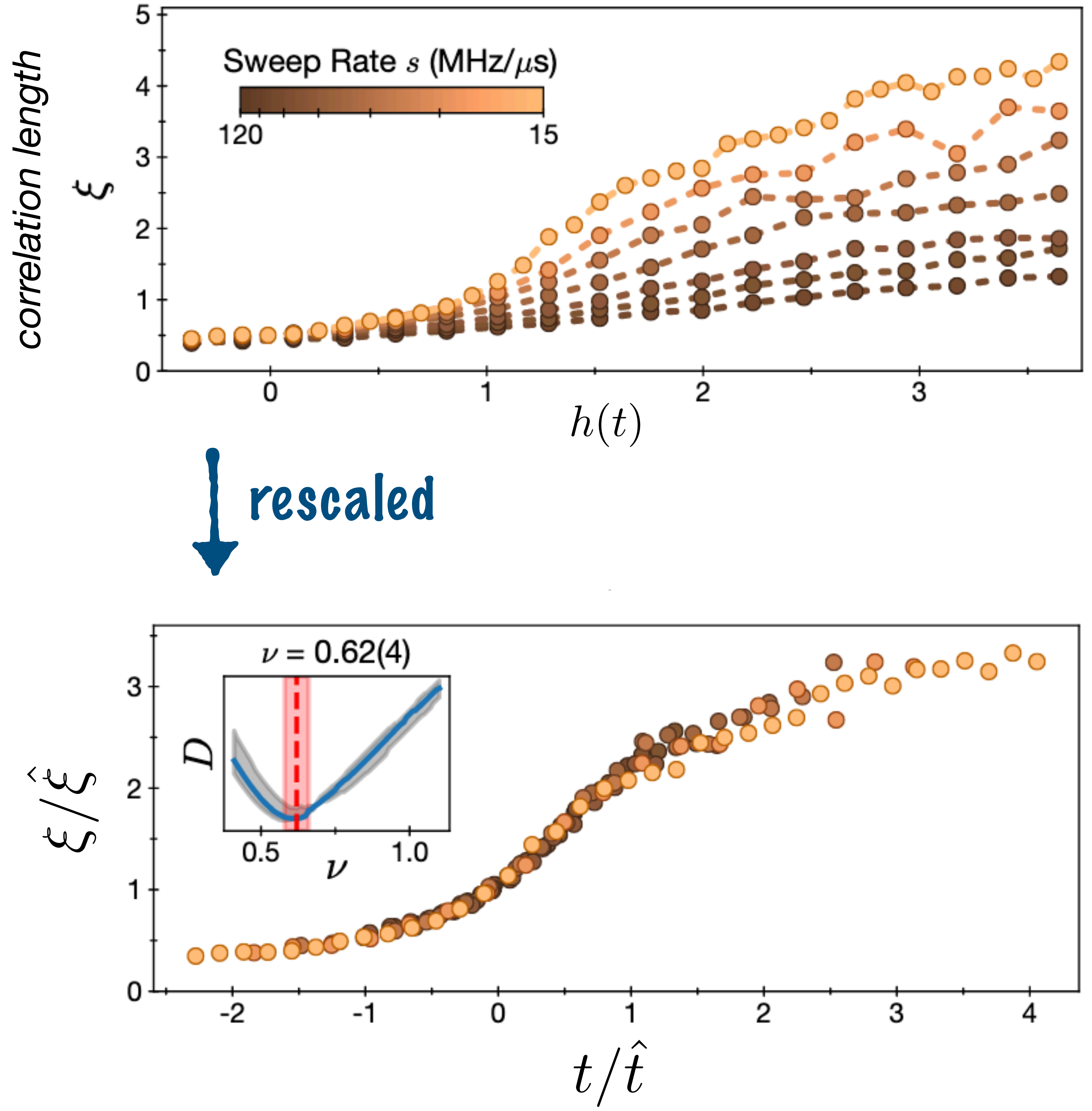
correlation function $C_{zz}(R) = \langle\psi|\sigma^z_{m,n}\sigma^z_{m+R,n}|\psi\rangle$



Scaling hypothesis: $O_L(t,R) = \hat{\xi}^{-\Delta_O} F_O(t/\hat{t}, R/\hat{\xi}, \hat{\xi}/L)$

Quantum simulation with Rydberg atom array

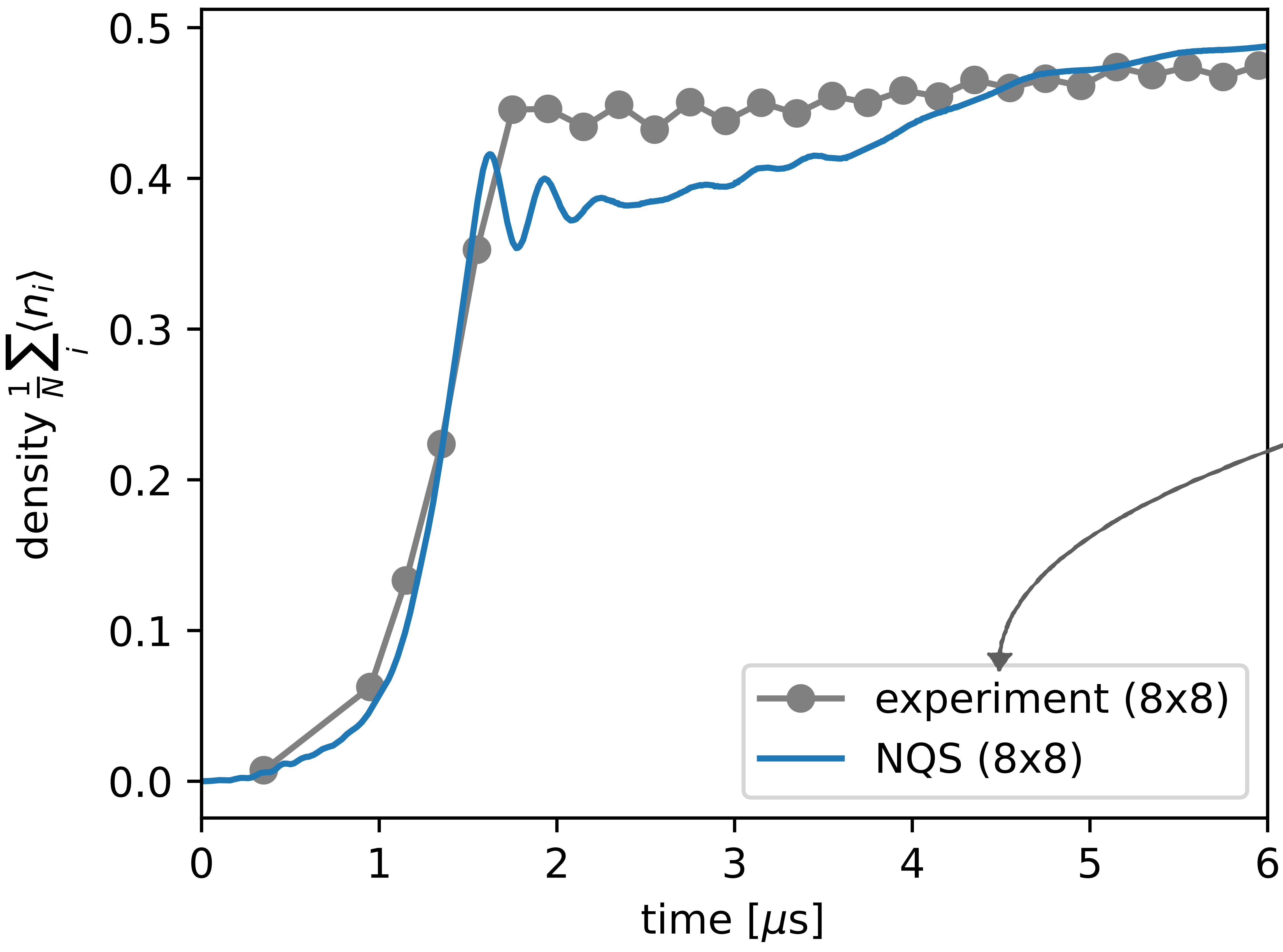
Ebadi *et al.*, *Nature* (2021)

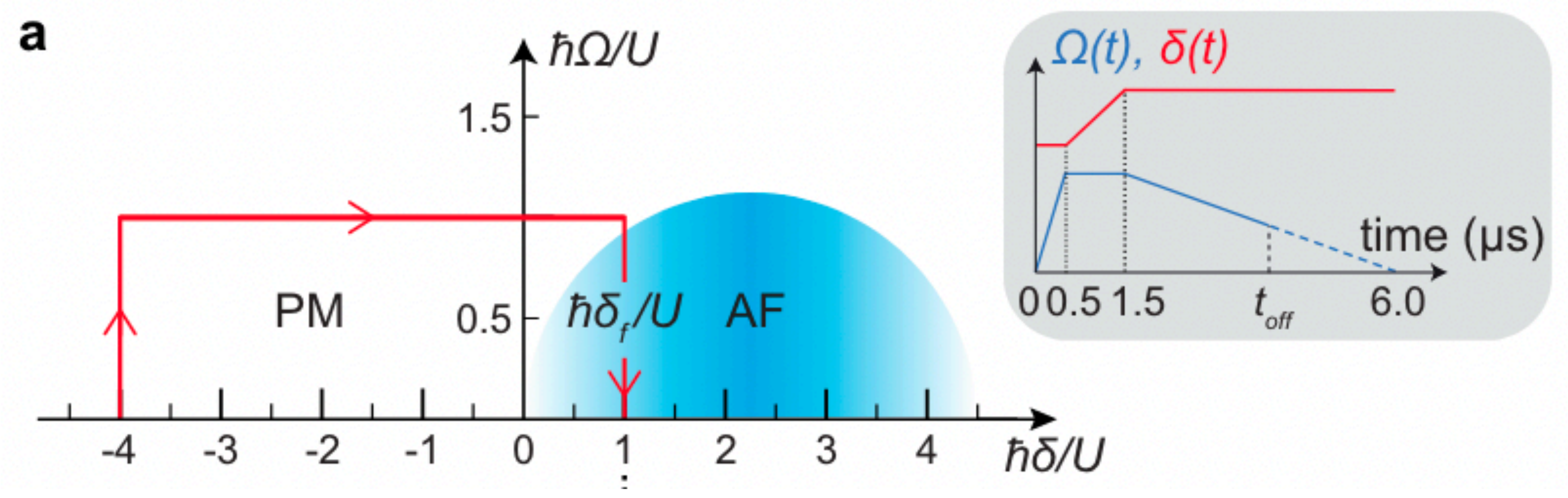


→ **Confirmation of non-equilibrium scaling hypothesis for a 2D quantum lattice model**

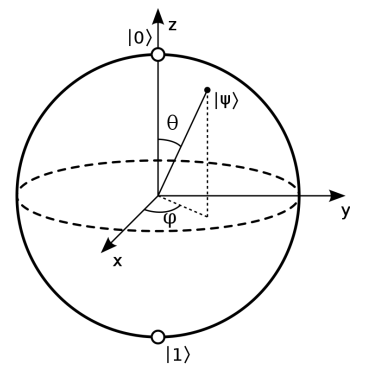
Outlook

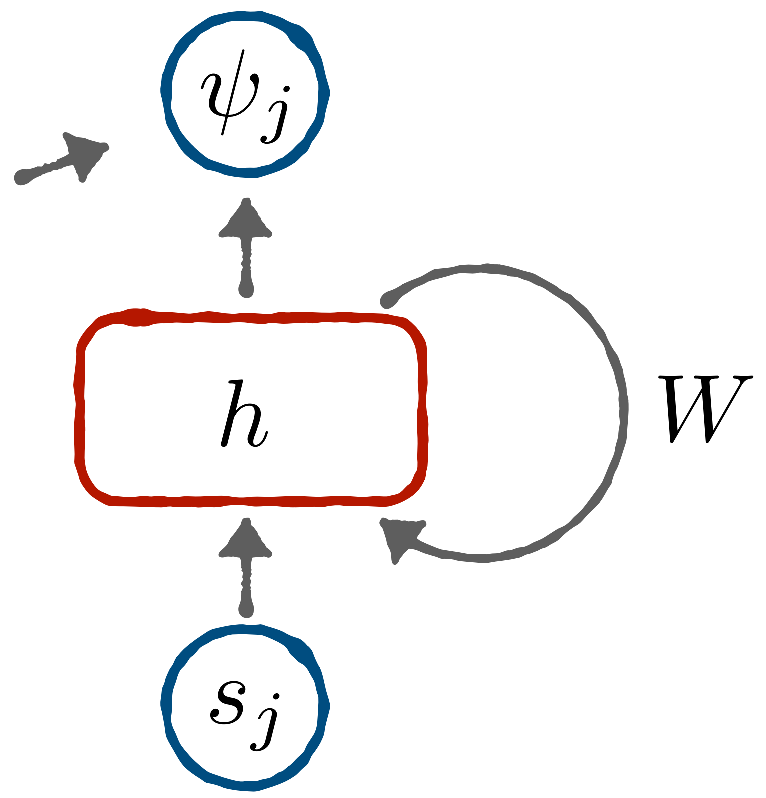
$$\hat{H}(t) = \frac{1}{2}\sum_i \Omega_i(t)\hat{\sigma}_i^x + \sum_i \left(\sum_{\langle i,j \rangle} \frac{U_0}{|r_{ij}|^6} - \frac{1}{2}\delta_i(t) \right)\hat{\sigma}_i^z + \sum_{\langle i,j \rangle} \frac{U_0}{|r_{ij}|^6}\hat{\sigma}_i^z\hat{\sigma}_j^z$$





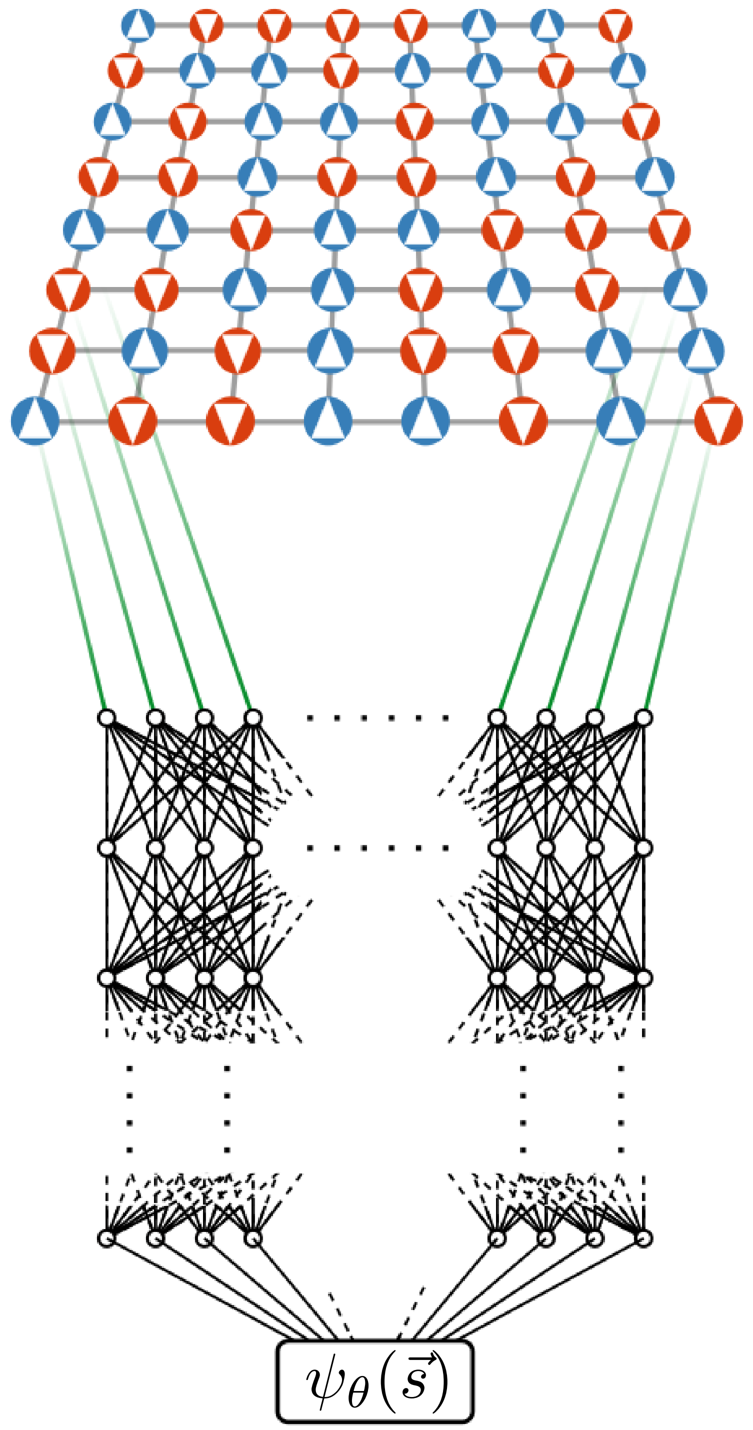
Scholl, …, Browaeys, *Nature* (2021)



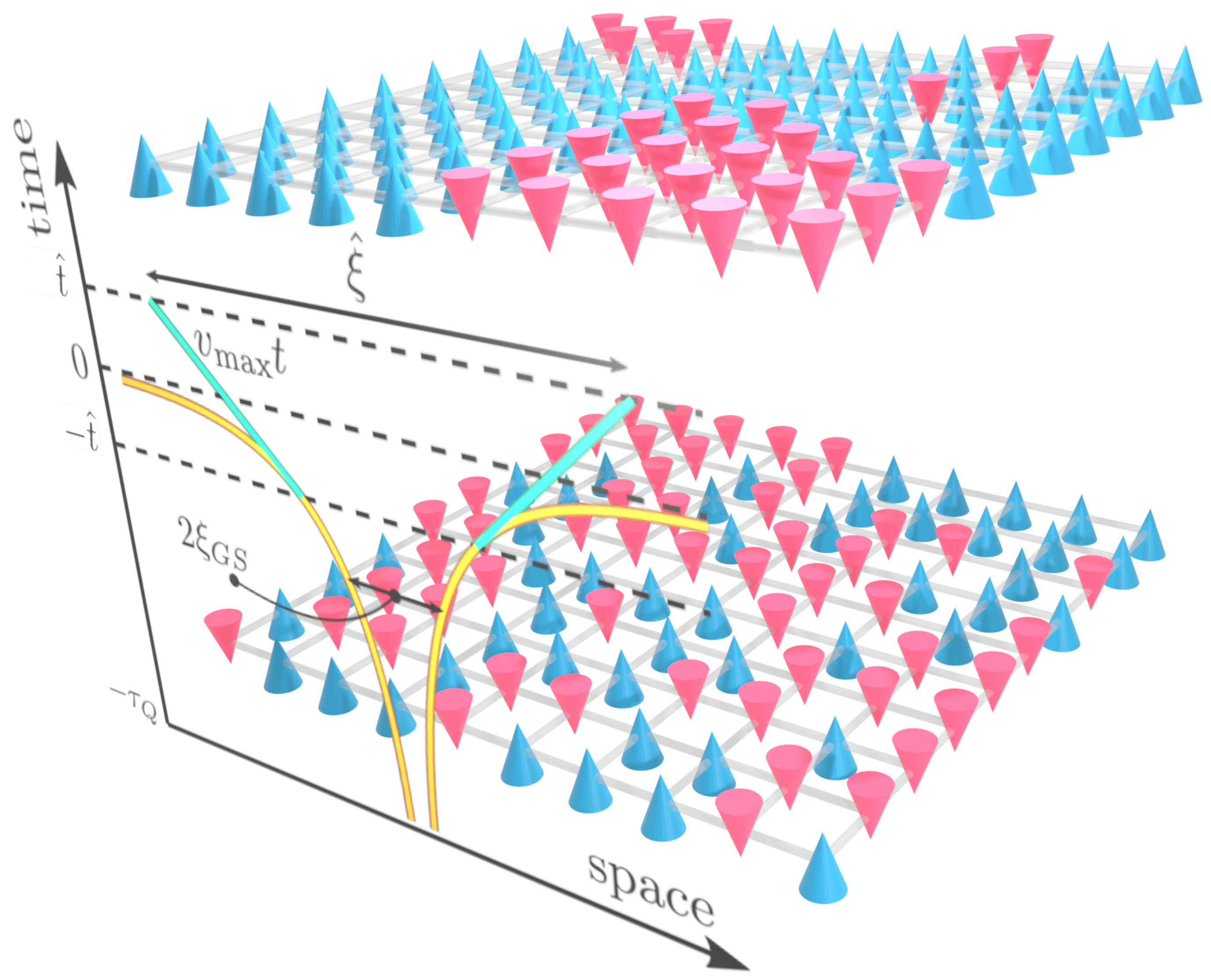


RNN + Bloch angles

Summary



🗒 *arXiv:2106.09046*



- **Neural quantum states** push capabilities to simulate non-equilibrium quantum matter
- Confirmation of **dynamical universality** in two-dimensional quantum lattice model




Markus Heyl — *Uni Augsburg*

Marek Rams, Jacek Dziarmaga — *Uni Krakow*

Wojciech Zurek — *Los Alamos Lab*

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