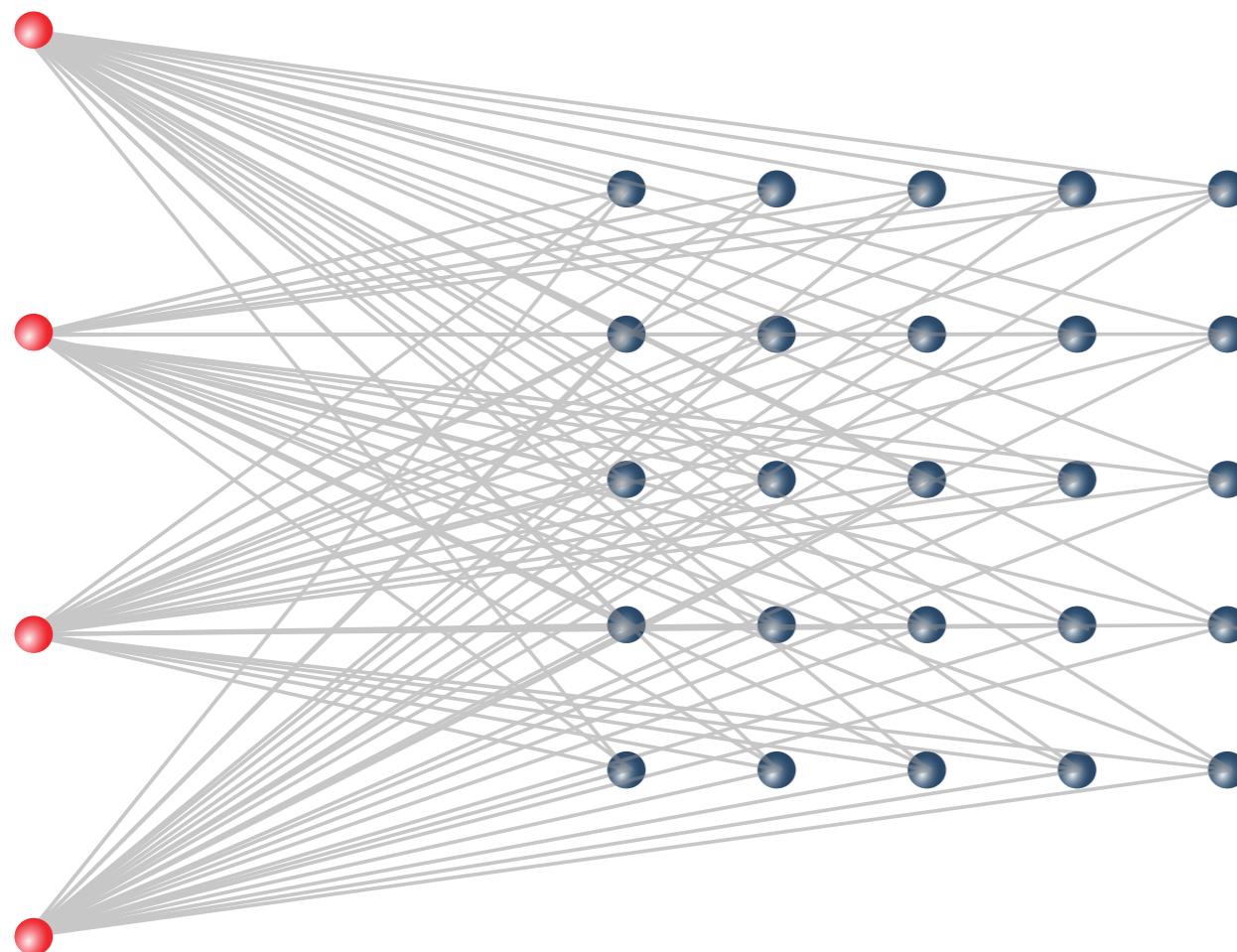


Neural-Network Approach to Dissipative Quantum Many-Body Dynamics



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Google

Quantum Many-Body Problem

size of Hilbert space exponential in number of subsystems

$$|\psi\rangle = \sum_{j_1, j_2, \dots, j_N=0}^1 c_{j_1, j_2, \dots, j_N} |j_1, j_2, \dots, j_N\rangle$$

$$|\langle j_1, j_2, \dots, j_N | \psi \rangle|^2 = |c_{j_1, j_2, \dots, j_N}|^2$$

probability distribution
 2^N possible events

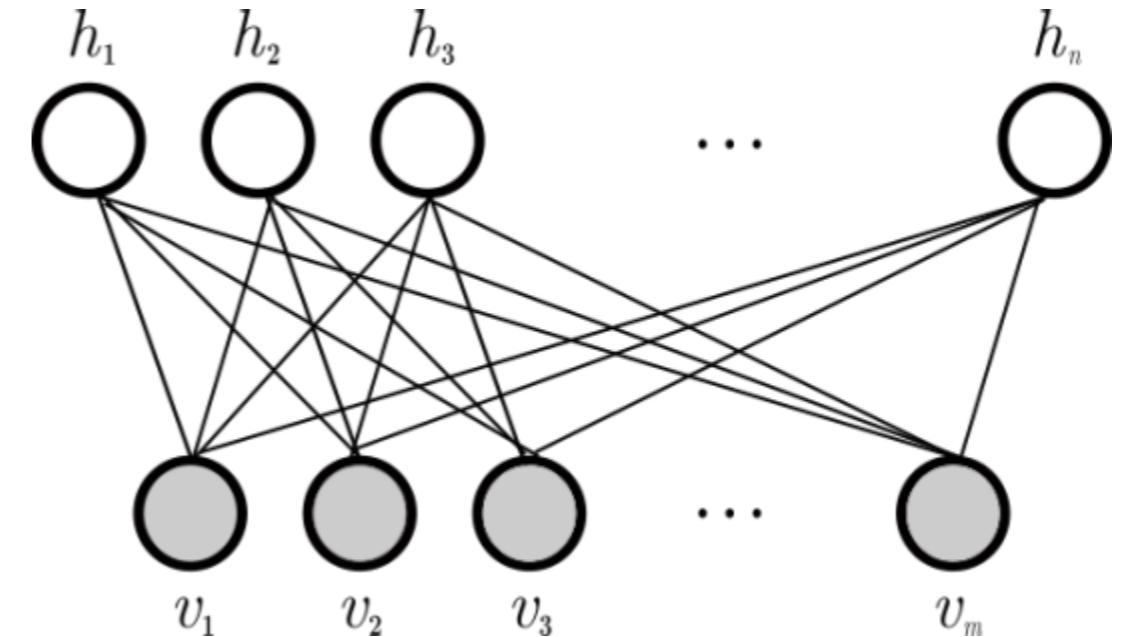
use stochastic generative neural netw. to model distribution
→ only specify network parameters (weights and biases)
→ can be more efficient

has been done for closed systems
this talk → open systems

Carleo and Troyer, Science 355, 602 (2017)
→ talk by Filippo Vicentini

Restricted Boltzmann Machines

neural network with 1 ‘visible’
and 1 ‘hidden’ layer



probability for configuration:

$$P(\vec{v}, \vec{h}) = \exp \left[\sum_{i,j} w_{ij} v_i h_j + \sum_j b_j h_j + \sum_i a_i v_i \right]$$

probability for
physical configuration
in thermal equilibrium:

$$P(\vec{v}) = \frac{e^{-\beta E(\vec{v})}}{Z}$$

sufficiently many hidden neurons
→ can train parameters such that:

$$\frac{e^{-\beta E(\vec{v})}}{Z} = \sum_{\{\vec{h}\}} P(\vec{v}, \vec{h})$$

Neural Network States

$$|\psi\rangle = \sum_{\vec{l}} c_{\vec{l}} |l_1, \dots, l_N\rangle$$

qubits: visible layer of neural network (N visible, M hidden)

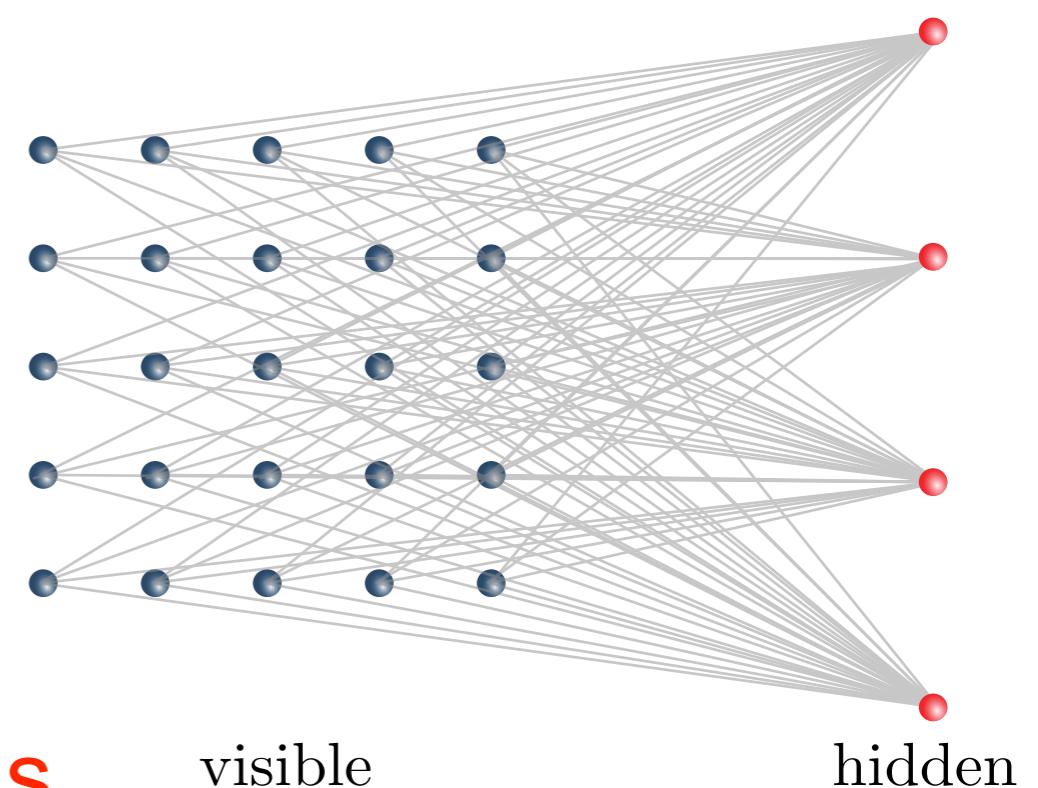
$$c_{\vec{l}} = \exp \left(\sum_{n=1}^N a_n l_n \right) \times \prod_{k=1}^M \cosh \left(b_k + \sum_{n=1}^N w_{k,n} l_n \right)$$

RBM summed over all configurations of hidden layer parametrization

$$c_{\vec{l}}(\alpha_1, \alpha_2, \dots, \alpha_{MN+M+N})$$

efficient if $MN + M + N \ll 2^N$

can model very nonlocal correlations



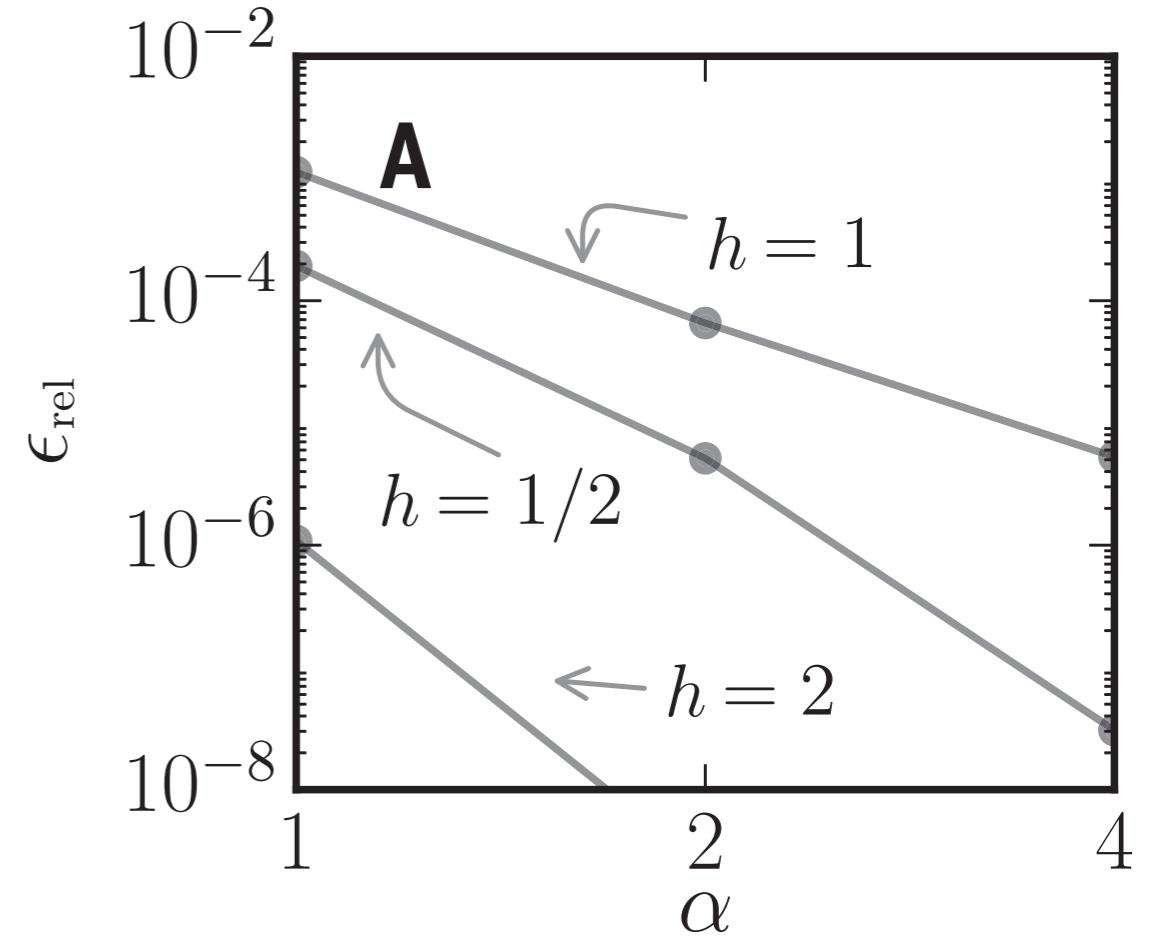
Ground State Approximation

find state with lowest energy
by optimizing the parameters

$$E = \min \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

→ phase diagram
→ quantum phase transitions

$$H_1 = -h \sum_i \sigma_i^x + \sum_{i,j} \sigma_i^z \sigma_j^z$$



similar accuracies as Tensor Networks in 1D
improves best known variational results for 2D

1D, $N = 80$
 $\alpha = M/N$

Quantum Dynamics

not only interested in ground states

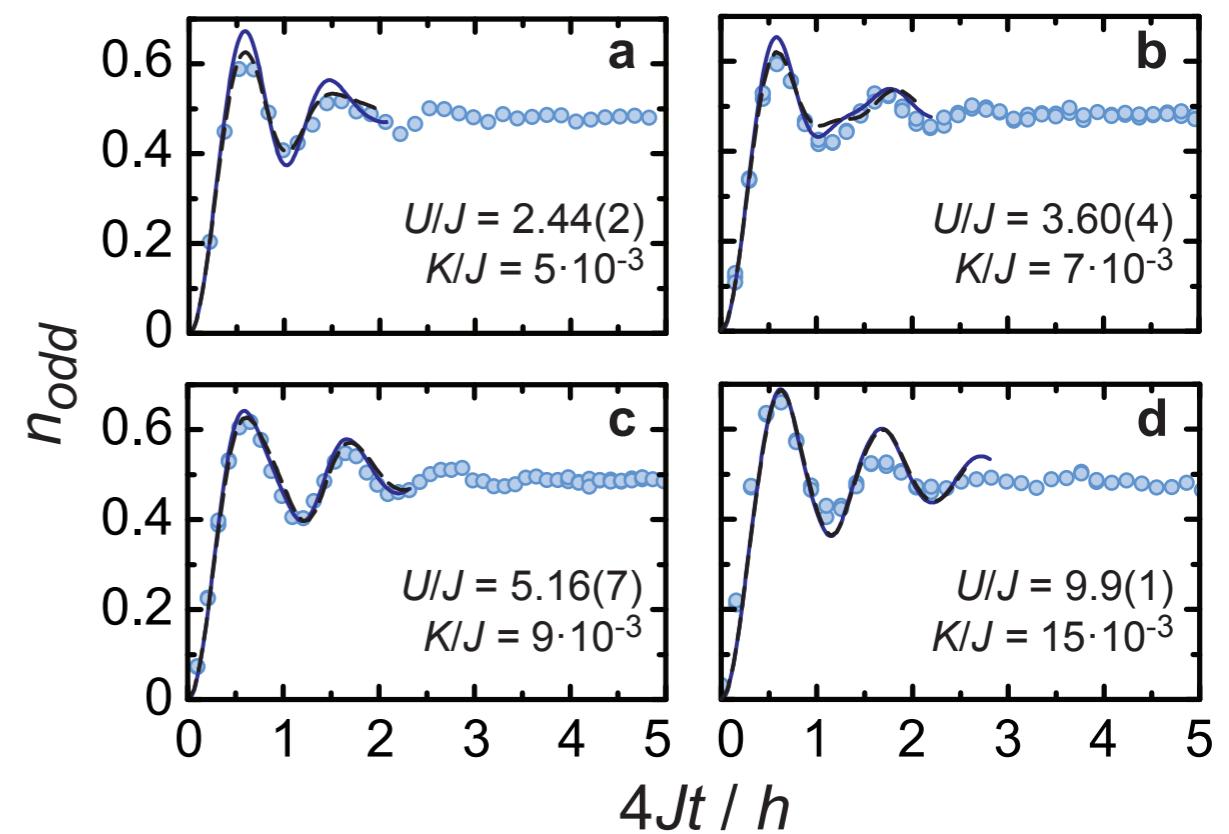
ground states often obey an area law (gapped systems)

- bound on entanglement entropy
- tensor networks become efficient

non-equilibrium dynamics

$$\partial_t |\psi\rangle = -iH|\psi\rangle$$

isolated quantum system
→ idealization



Open Quantum Systems

systems we investigate are never perfectly isolated

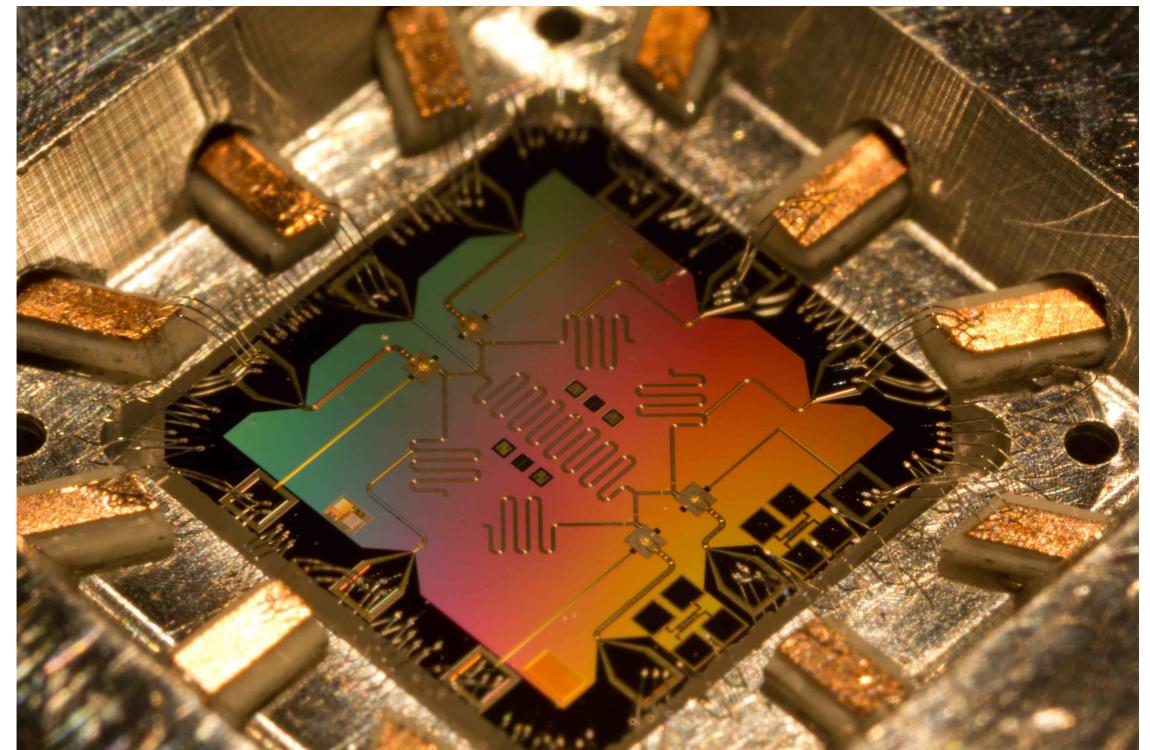


we investigate this

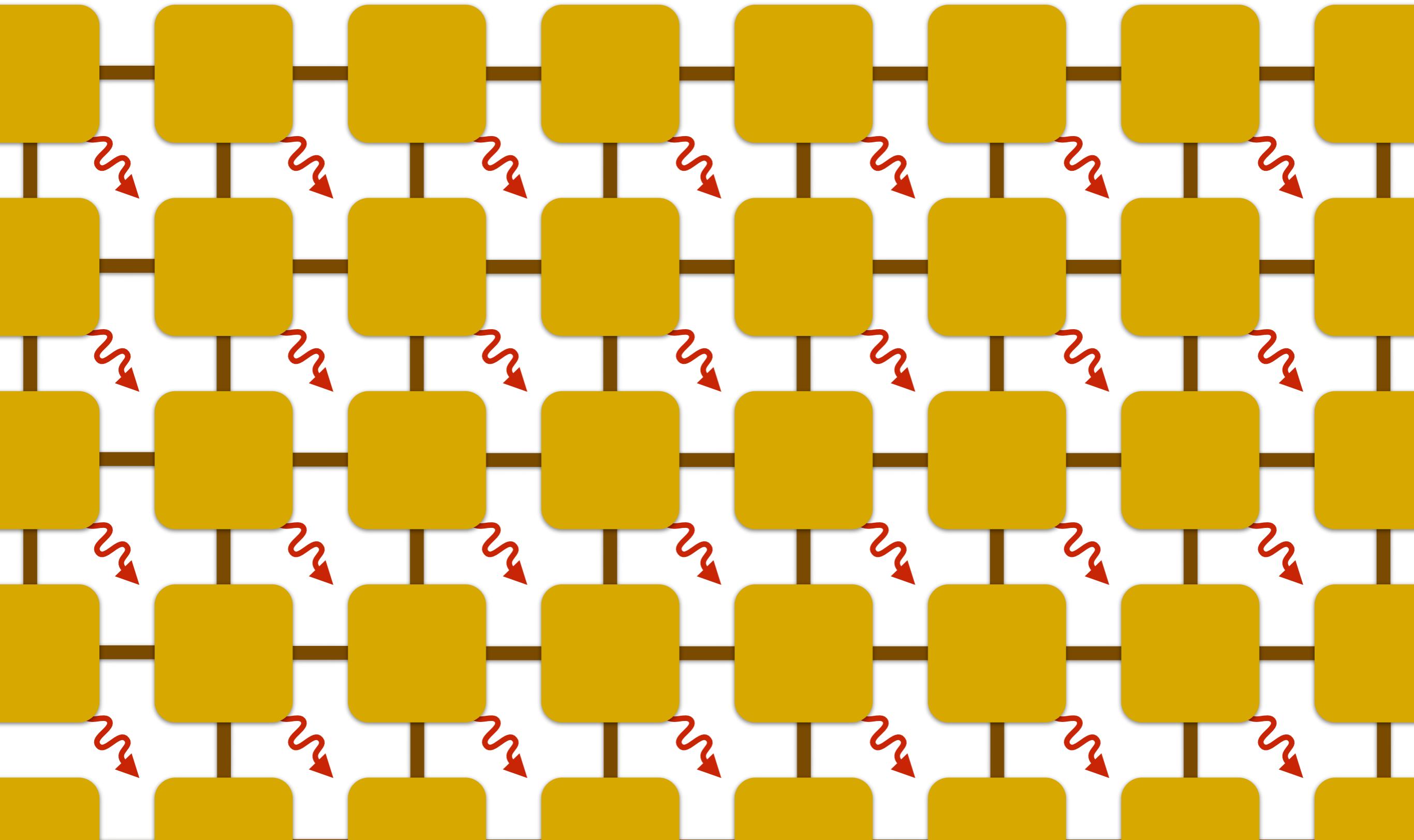
bi-partite quantum system
typically entangled
→ system in mixed state

$\dim(\mathcal{H})^2$ matrix elements

→ even more demanding than pure states

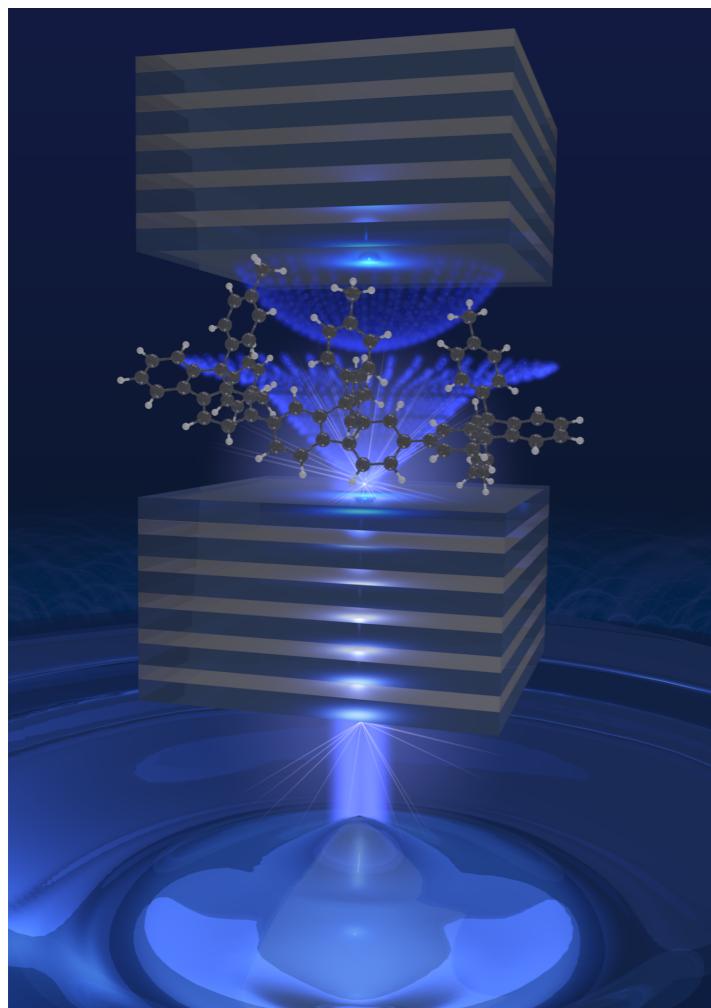


Dissipative Lattice Systems



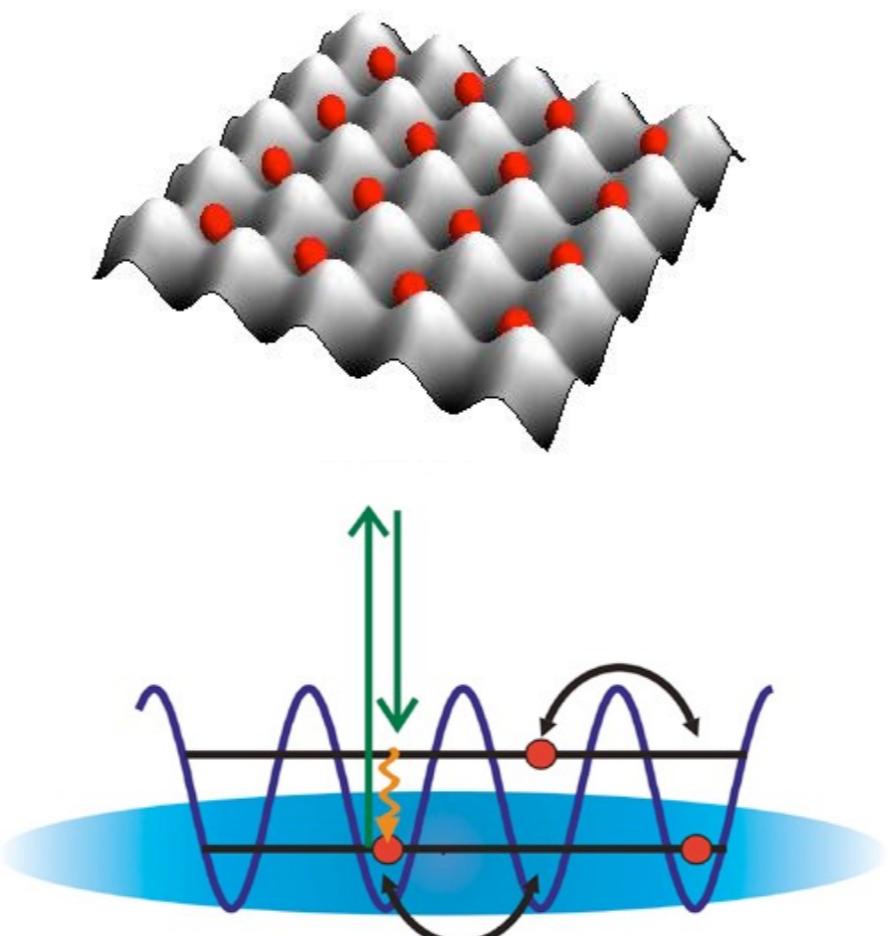
Driven-Dissipative Systems

exciton-polariton
condensation



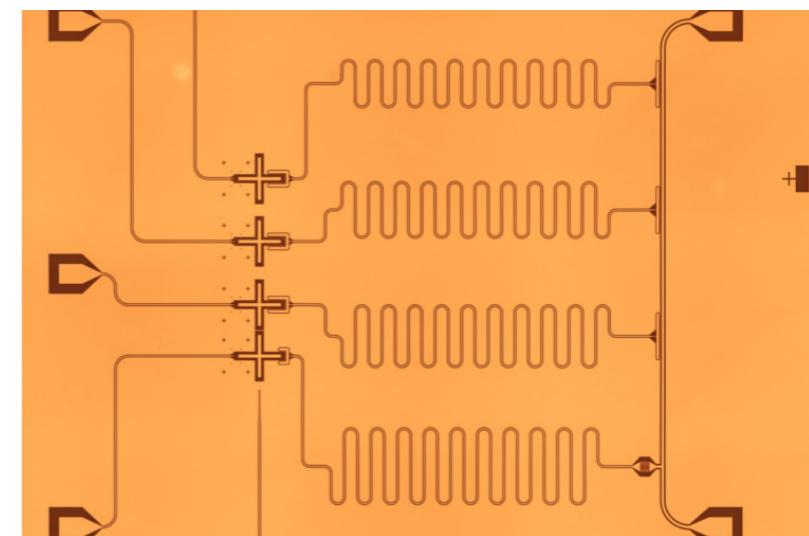
Kasprzak et al.,
Nature **443**, 409 (2006)
Sieberer et al.,
Rep. Prog. Phys. **79**, 096001 (2016)

optical lattices



Diehl et al.,
Nat. Phys. **4**, 878 (2008)
Baumann et al.,
Nature **464**, 1301 (2010)

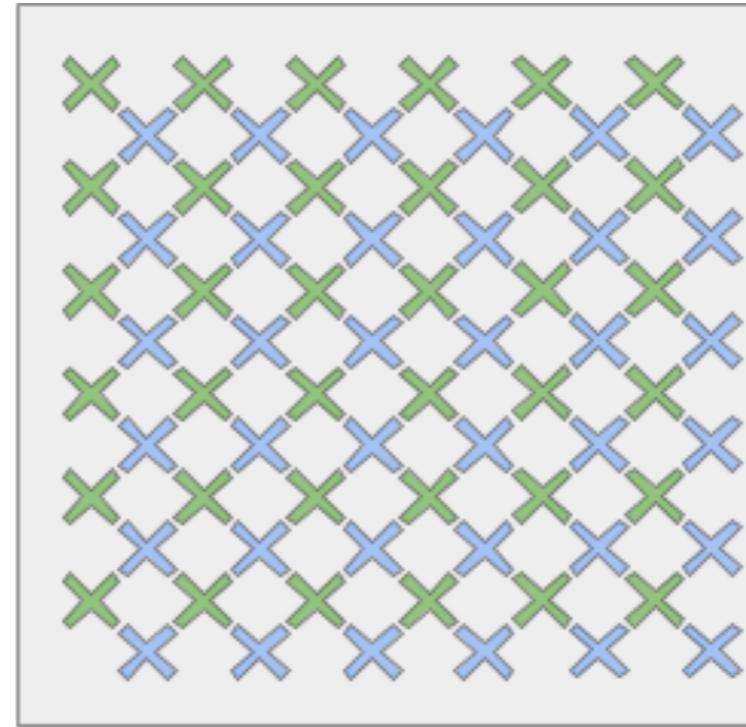
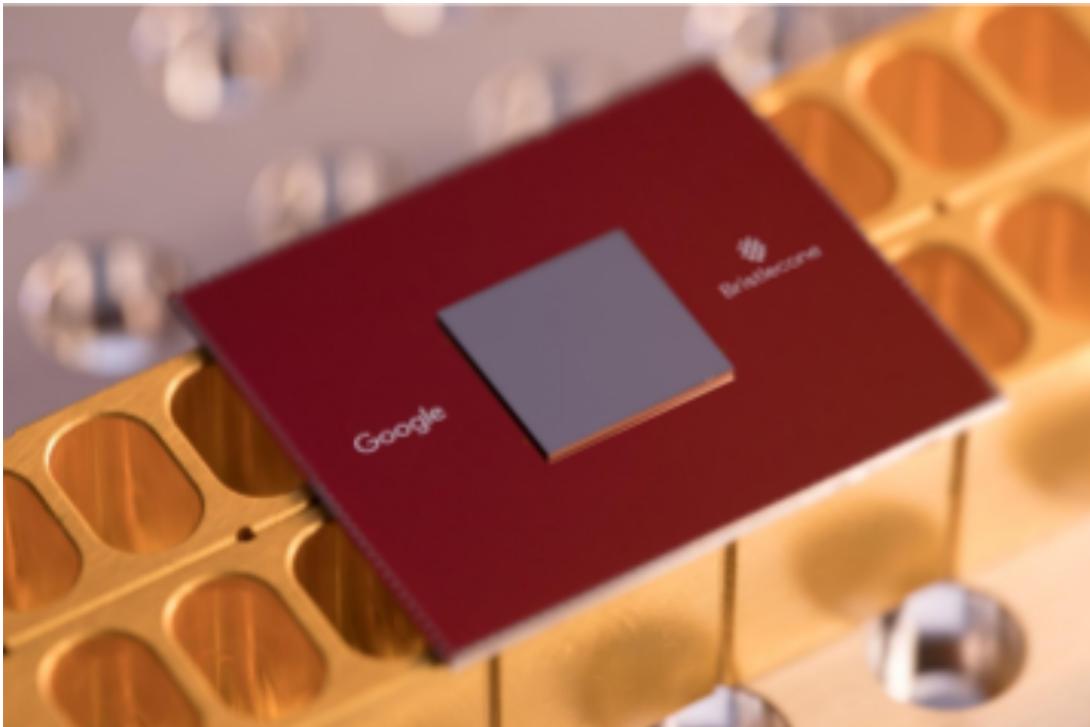
superconducting
circuits



Hartmann,
J. Opt. **18**, 104005 (2016)
Ma, et al.,
Nature **566**, 51–57, (2019)

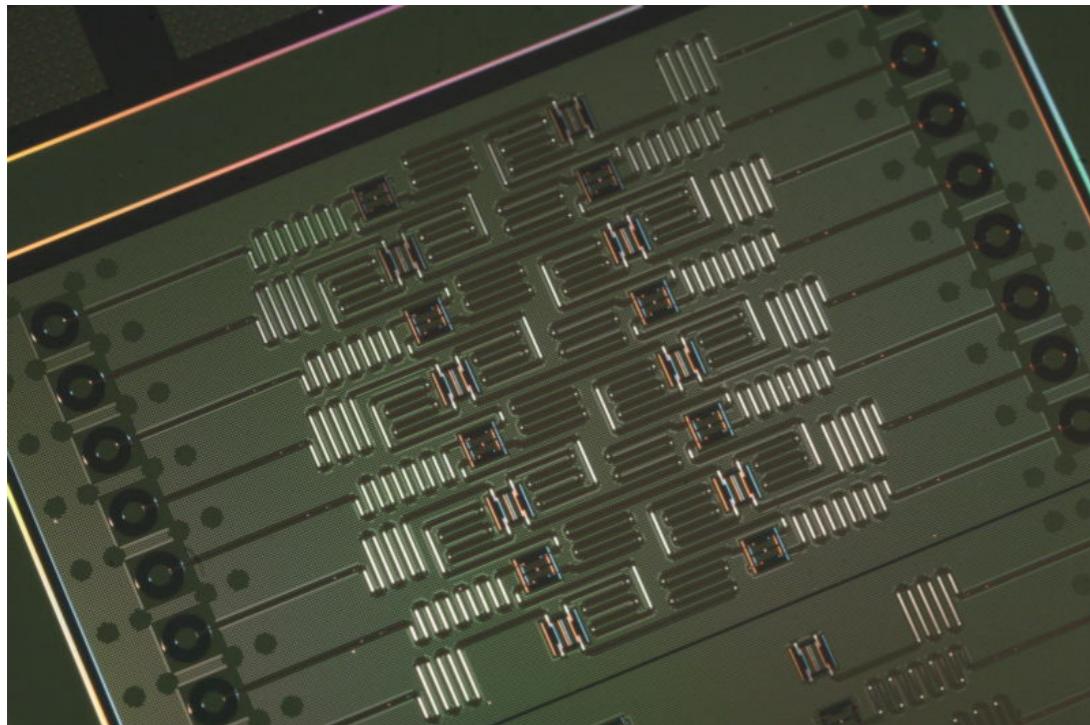
→ interesting quantum
many-body physics
→ phase transitions
between steady states?

Quantum Computers & Dissipation



2D quantum
lattice-system

dissipation:
 T_1 and T_2



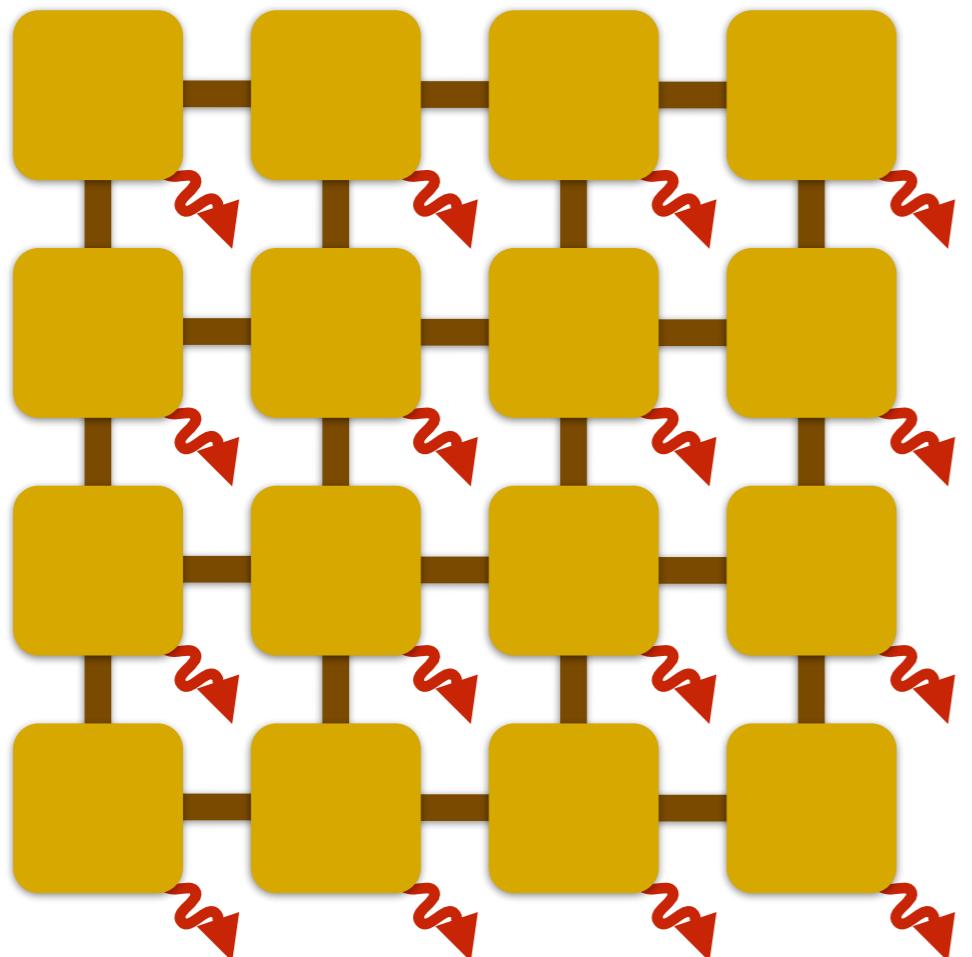
will soon reach size that
can't be modeled exactly

PEPS: challenging,
no efficient
contraction

Kshetrimayum, Weimer & Orus,
Nat. Commun. 8, 1291 (2017)

need better suited method

Dissipative Quantum Many-Body Problem



unitary dynamics of system
could also be gate sequence

$$\dot{\rho} = -i[H, \rho]$$

$$+ \sum_j \frac{\gamma}{2} (2\sigma_j^- \rho \sigma_j^+ - \{\sigma_j^+ \sigma_j^-, \rho\})$$

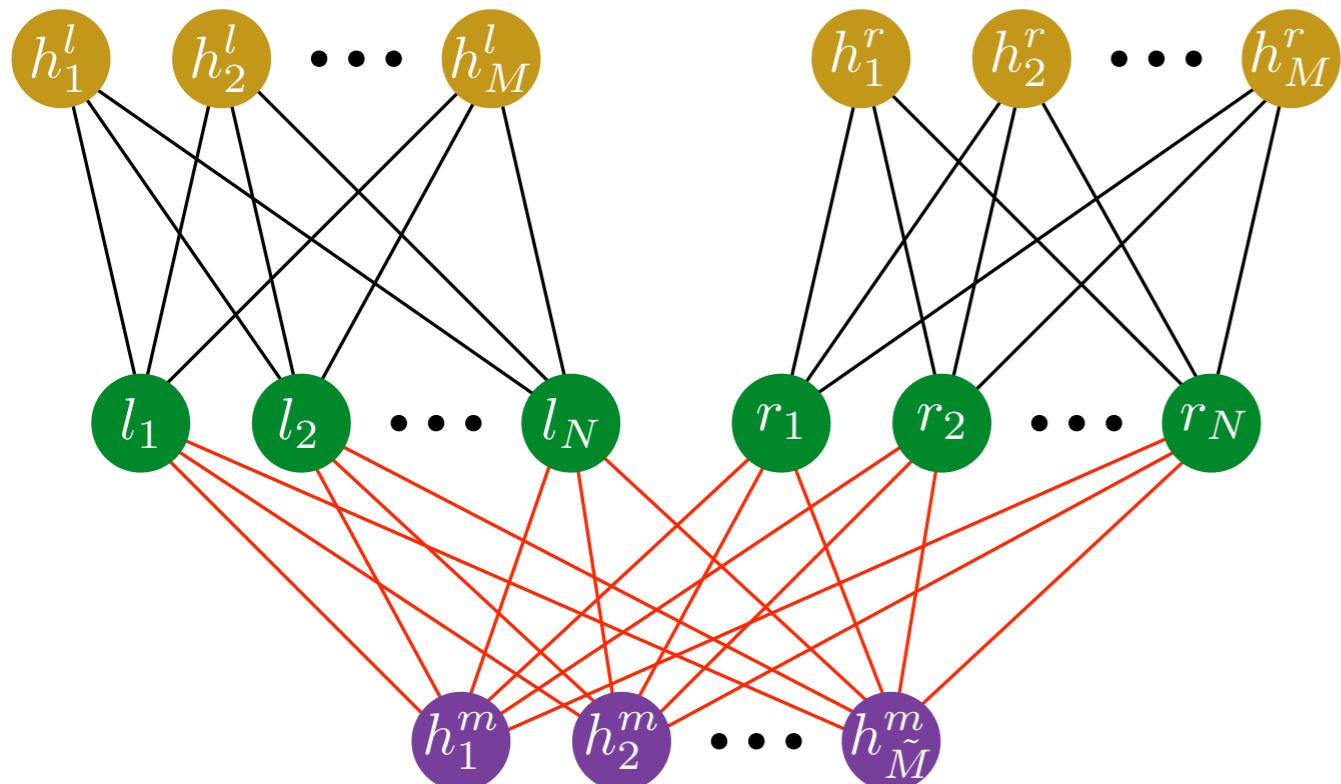
dissipation

$$\partial_t \vec{\rho} = \mathcal{L} \vec{\rho}$$

ρ exceedingly many degrees of freedom 2^{2N}

Neural Network Density Matrices

$$\hat{\rho} = \sum_{l_1, \dots, l_N, r_1, \dots, r_N=0}^1 \rho_{\vec{l}, \vec{r}} |l_1\rangle\langle r_1| \otimes \cdots \otimes |l_N\rangle\langle r_N|$$



parametrization

$$\rho_{\vec{l}, \vec{r}}(\alpha_1, \alpha_2, \dots, \alpha_n)$$

$\rho_{\vec{l}, \vec{r}}$: visible layer of
restricted Boltzmann
machine

$$\rho_{\vec{l}, \vec{r}} = \sum_{\vec{h}^m} \langle \vec{l}, \vec{h}^m | \psi \rangle \langle \psi | \vec{r}, \vec{h}^m \rangle$$

$$\rho^\dagger = \rho$$

ρ positive semi-definite

Stochastic Reconfiguration

$$\dot{\rho} = -i[H, \rho] + \frac{\gamma}{2} \sum_{j=1}^N (2\sigma_j^- \rho \sigma_j^+ - \sigma_j^+ \sigma_j^- \rho - \rho \sigma_j^+ \sigma_j^-)$$

$\partial_t \vec{\rho} = \mathcal{L} \vec{\rho}$ many-body master equation

$\vec{\rho}(\alpha_1, \alpha_2, \dots, \alpha_n)$ parameterization

$$\partial_t \vec{\rho} = \sum_k \dot{\alpha}_k O_k \vec{\rho} \quad [O_k]_{\vec{l}, \vec{r}} = \frac{\partial}{\partial \alpha_k} \ln(\rho_{\vec{l}, \vec{r}})$$

minimize:

$$\delta = \left\| \sum_k \dot{\alpha}_k O_k \vec{\rho} - \mathcal{L} \vec{\rho} \right\|_2^2$$

$$\Rightarrow \sum_p S_{k,p} \dot{\alpha}_p = f_k$$

coupled ODEs for α_k

→ network training

Monte Carlo and Sampling

$$\sum_p S_{k,p} \dot{\alpha}_p = f_k$$

requires full
density matrix

$$S_{k,p} = \vec{\rho}^\dagger O_k^\dagger O_p \vec{\rho} + \vec{\rho}^\dagger O_p^\dagger O_k \vec{\rho}$$
$$f_k = \vec{\rho}^\dagger O_k^\dagger \mathcal{L} \vec{\rho} + \vec{\rho}^\dagger \mathcal{L}^\dagger O_k \vec{\rho}$$

$$[O_k]_{\vec{l}, \vec{r}} = \frac{\partial}{\partial \alpha_k} \ln(\rho_{\vec{l}, \vec{r}})$$

$$\vec{\rho}^\dagger O_k^\dagger \mathcal{L} \vec{\rho} = \sum_{\vec{l}_1, \vec{r}_1} \sum_{\vec{l}_2, \vec{r}_2} |\rho_{\vec{l}_1, \vec{r}_1}|^2 \frac{\partial \ln(\rho_{\vec{l}_1, \vec{r}_1}^*)}{\partial \alpha_k} \frac{\mathcal{L}_{\vec{l}_1, \vec{r}_1; \vec{l}_2, \vec{r}_2} \rho_{\vec{l}_2, \vec{r}_2}}{\rho_{\vec{l}_1, \vec{r}_1}}$$

calculate by sampling from: $p(\vec{l}, \vec{r}) = |\rho_{\vec{l}, \vec{r}}|^2$

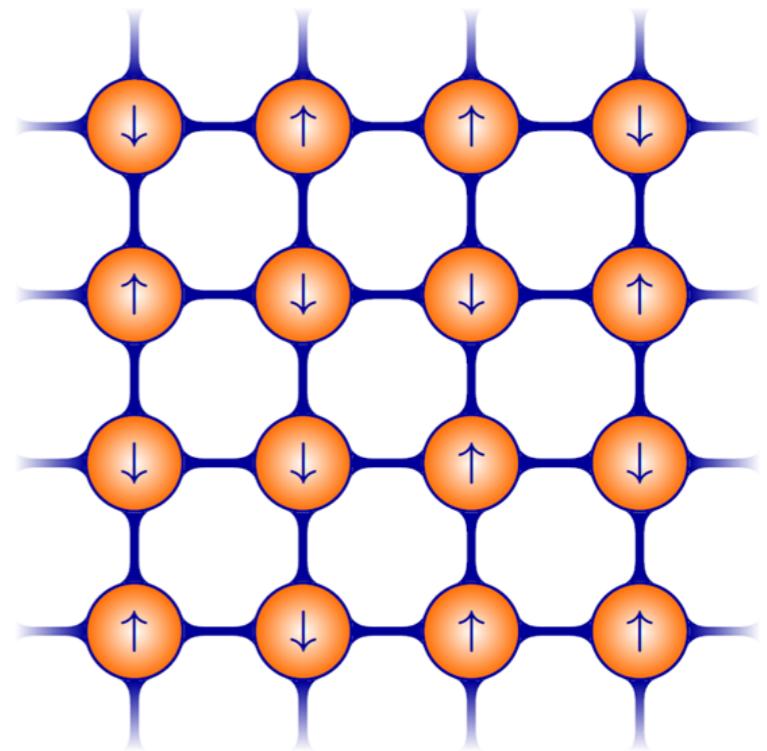
Metropolis
algorithm

never need full density matrix

works in 2d

Un-isotropic Heisenberg Lattice with Dissipation

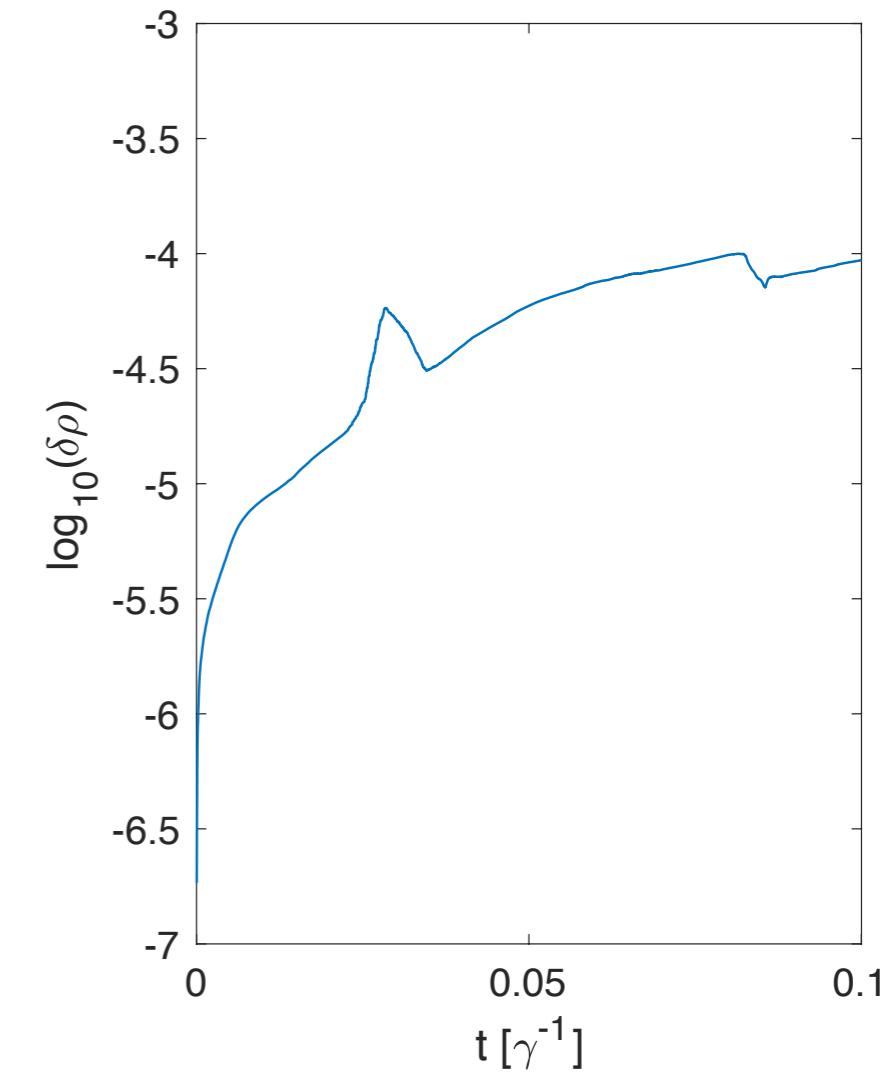
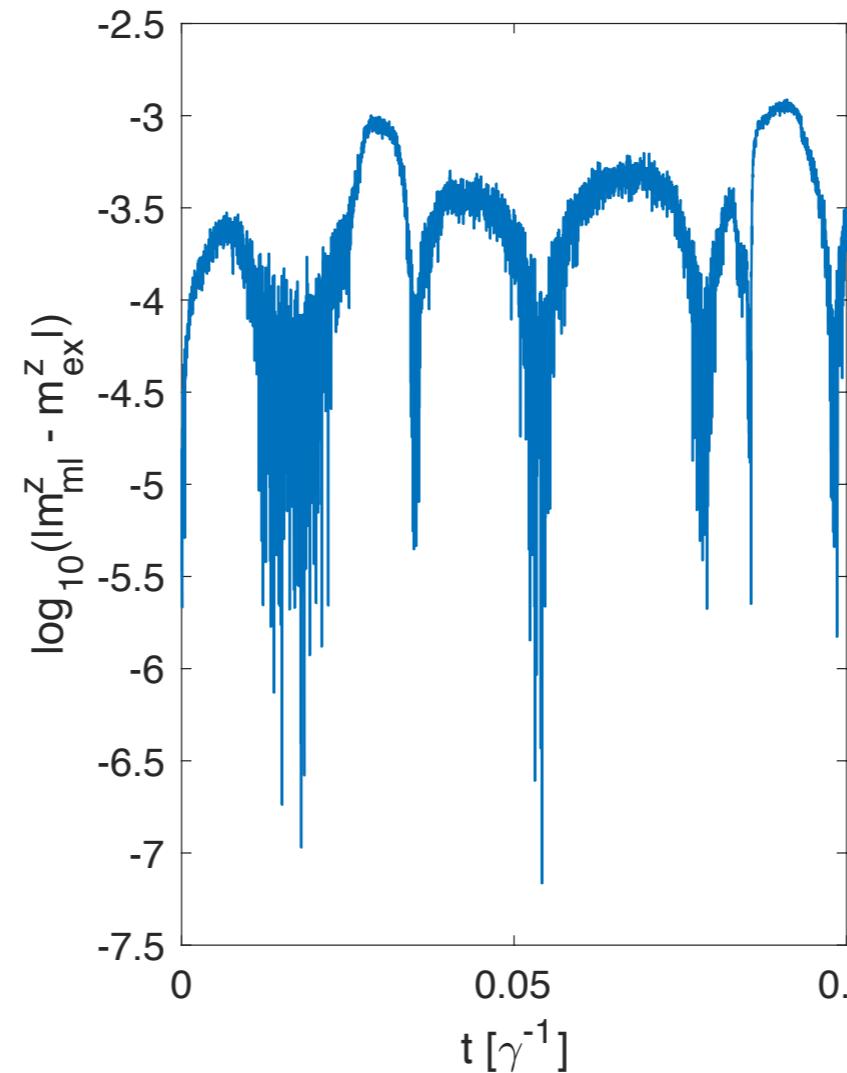
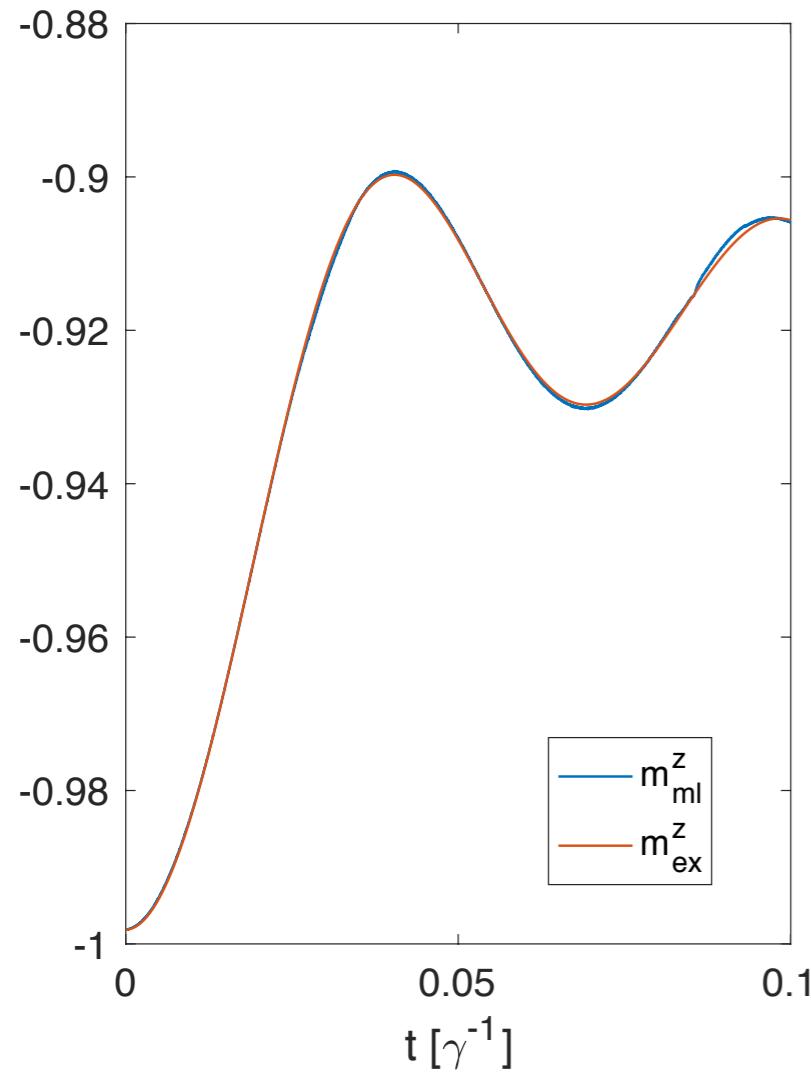
$$H = \sum_{j=1}^N B\sigma_j^z + \sum_{\langle j,l \rangle} \sum_{a=x,y,z} J_a \sigma_j^a \sigma_l^a$$



$$\dot{\rho} = -[H, \rho] + \frac{\gamma}{2} \sum_{j=1}^N (2\sigma_j^- \rho \sigma_j^+ - \sigma_j^+ \sigma_j^- \rho - \rho \sigma_j^+ \sigma_j^-)$$

First Results: Dynamics

chain of 5 spins with periodic boundary conditions



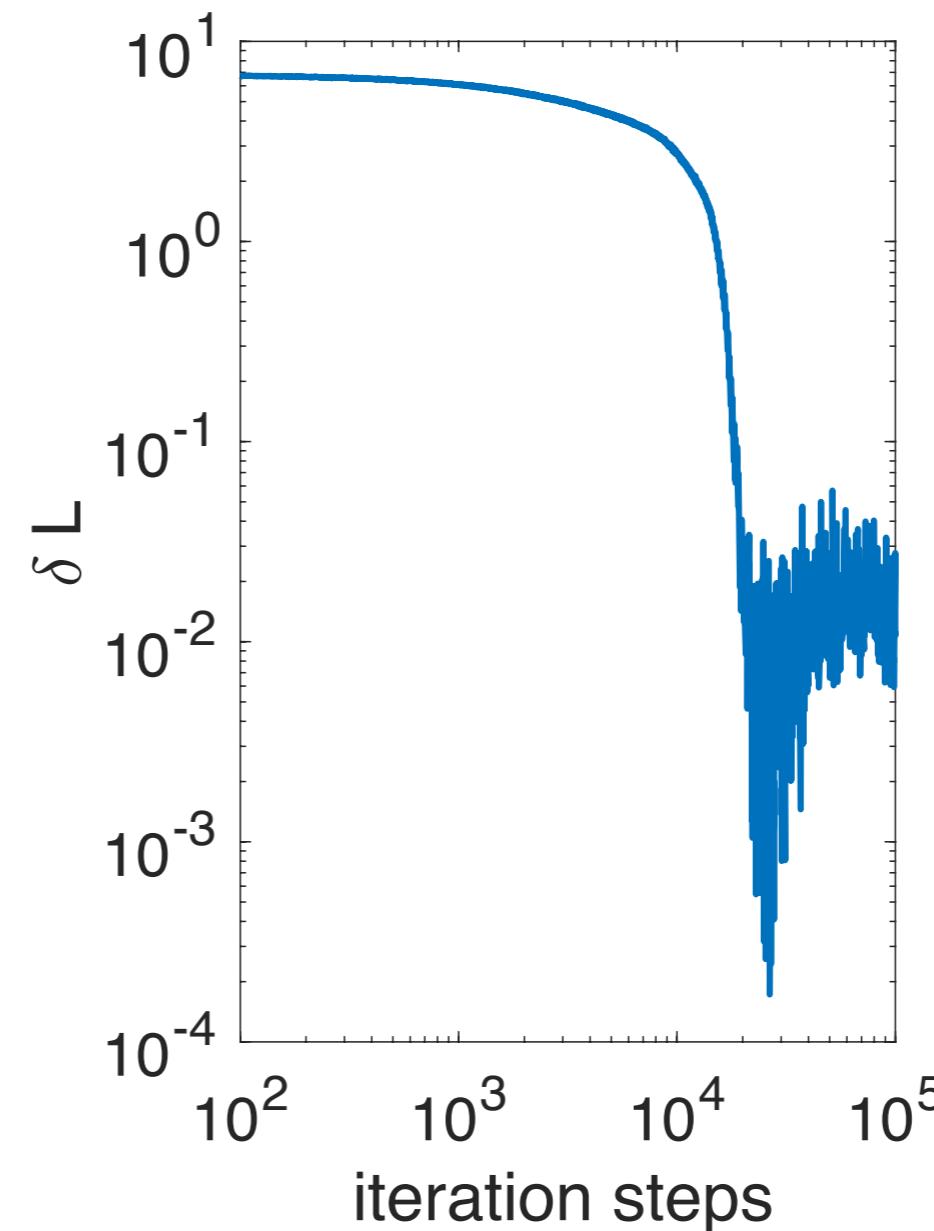
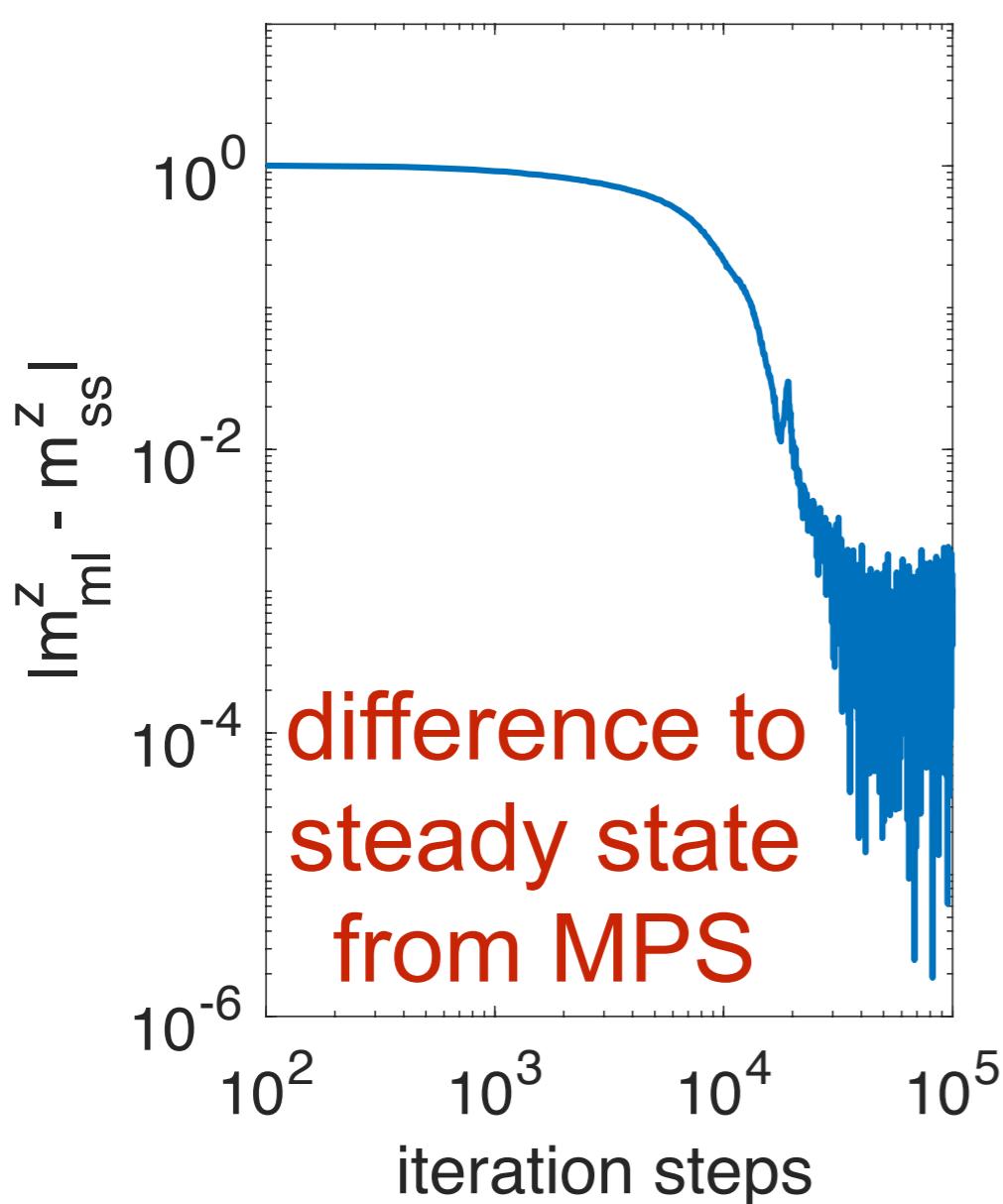
40 hidden neurons
sample size 200k

$B = 10\gamma, J_x = 20\gamma, J_y = 0, J_z = 10\gamma$

$$\delta\rho = \frac{1}{2^{2N}} \sqrt{\sum_{j,l} |\rho_{j,l} - \rho_{j,l}^e|^2}$$

First Results: Steady States

chain of 16 spins with open boundary conditions



tests whether
 $\mathcal{L}\rho = 0$
computed
from samples

36 hidden neurons, sample size 200k

$$B = \gamma, \quad J_x = 0.1 \gamma, \quad J_y = J_z = 0$$

New Group @ FAU

I'm moving to:
Here!



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for the science of light

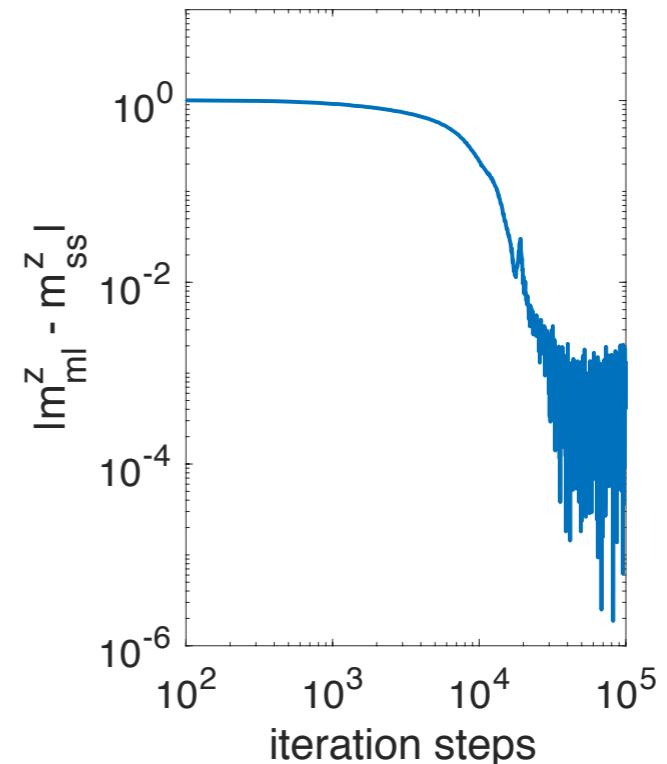
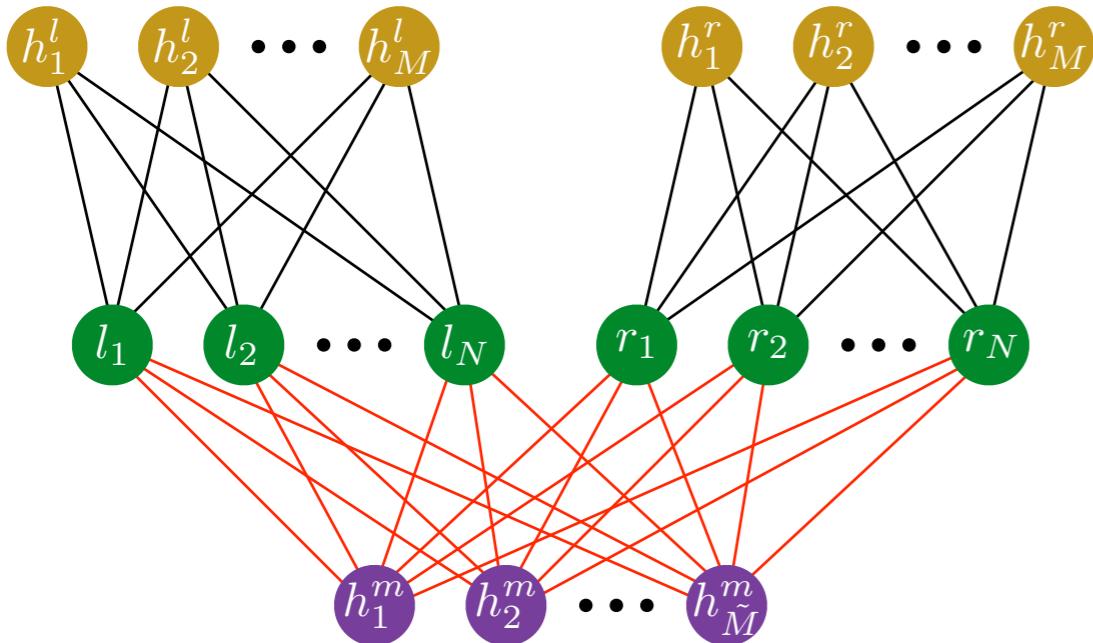
associated
with

Postdoc and PhD positions available:

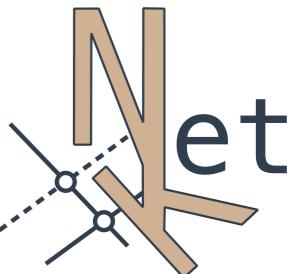
- ▶ machine learning in quantum science
- ▶ dissipative quantum many body systems
- ▶ superconducting qubits architectures
- ▶ near term applications of NISQ hardware

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Thank you for listening



Hartmann & Carleo, arXiv:1902.05131



- improve code, integration into NetKet: www.netket.org
- different networks, complex variational parameters,...