YITP workshop “Recent progress in theoretical physics based on quantum information theory”

Advancing Variational Algorithms for Quantum Many-body Problems

Nobuyuki Yoshioka (UTokyo)

2021.03.02

東京大学
THE UNIVERSITY OF TOKYO

Collaborators

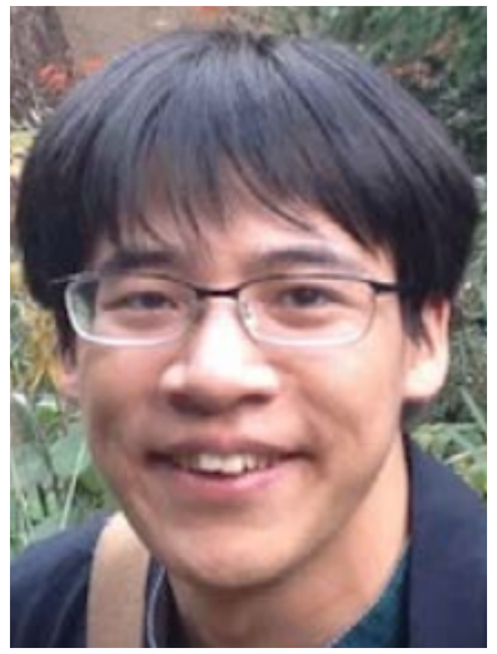
Variational simulation of open quantum system

[1] NY & R. Hamazaki, PRB 99, 214306 (2019).

[2] NY, Y.O.Nakagawa, K.Mitarai, K. Fujii, PRR 2, 043289 (2020).

Neural-net simulation of finite temperature state

[3] Y. Nomura, NY, F. Nori, arXiv:2103.04971



Ryusuke Hamazaki
(RIKEN)

Franco Nori
(RIKEN)

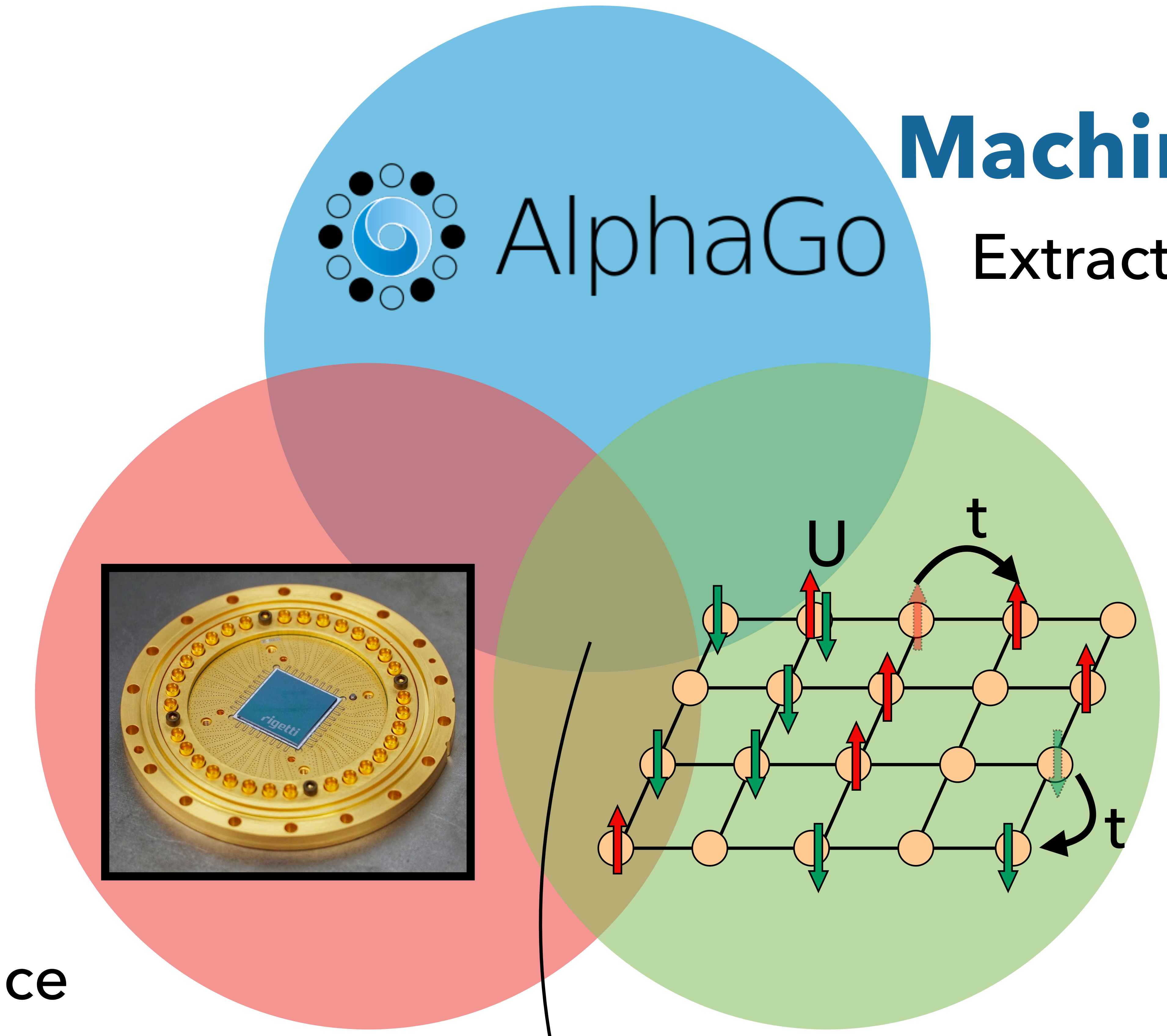
Yusuke Nomura
(RIKEN)

Yuya O. Nakagawa
(QunaSys)

Kosuke Mitarai
(Osaka Univ.)

Keisuke Fujii
(Osaka Univ.)

Variational simulation as question at the crosspoint



Machine Learning

Extracting patterns from classical data

Quantum Technology

Information processing
using quantum interference

Condensed-matter physics

Exotic phenomena from
many-body correlation

How to tame the "curse of dimensionality"?

(Explosive increase in Hilbert/feature space prohibits exact solutions)

Variational simulation of many-body problems

Key elements in variational algorithm

1. Find appropriate “cost function” to map full-Hilbert space operation in parameter space
2. Find suitable parametrization that captures the quantum state

Linear equation to be solved

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

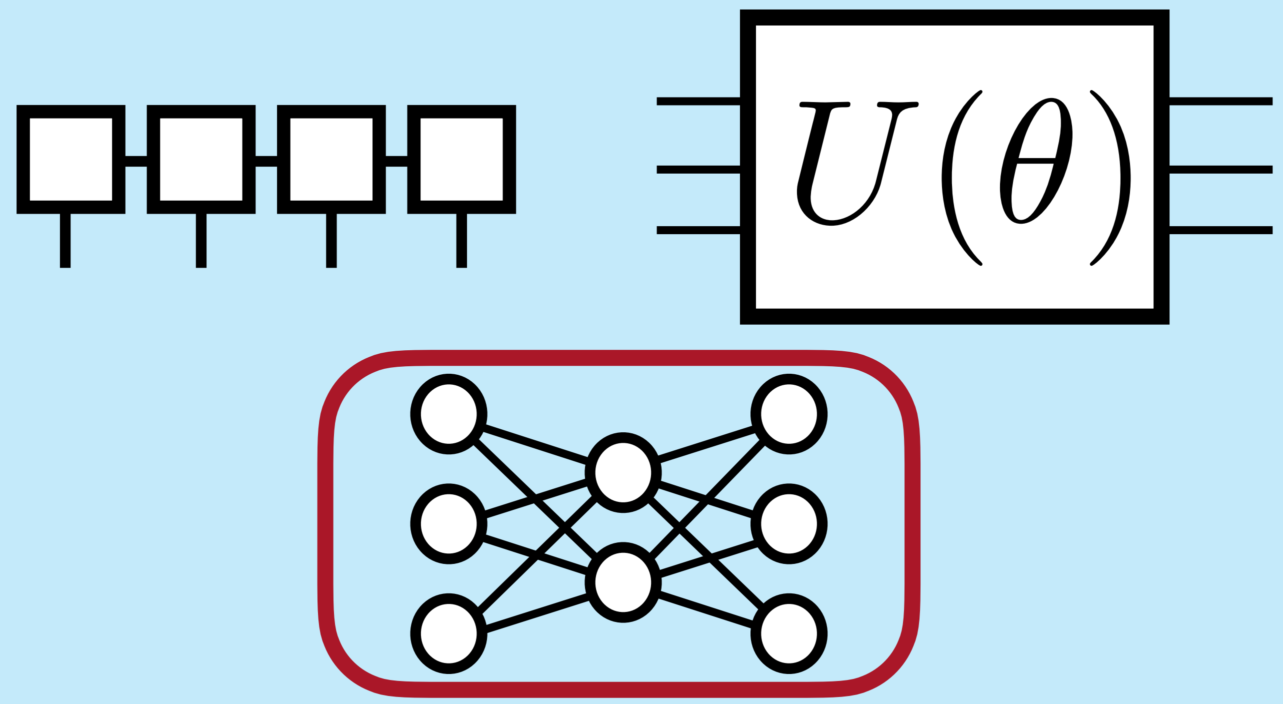
Exponential cost for exact solution

1. Appropriate “cost function”

$$\widetilde{E}_{GS} = \underset{\theta}{\operatorname{argmin}} \frac{\langle\Psi_\theta|\hat{H}|\Psi_\theta\rangle}{\langle\Psi_\theta|\Psi_\theta\rangle}$$

2. Choose GS approximant Ψ_θ

(Hopefully) polynomial parameters



Static property

- Symmetry breaking
- Ordering

Dynamic property

- Response func.
- Thermalization

Neural Networks as variational ansatz

Carleo&Troyer Science 355('17)

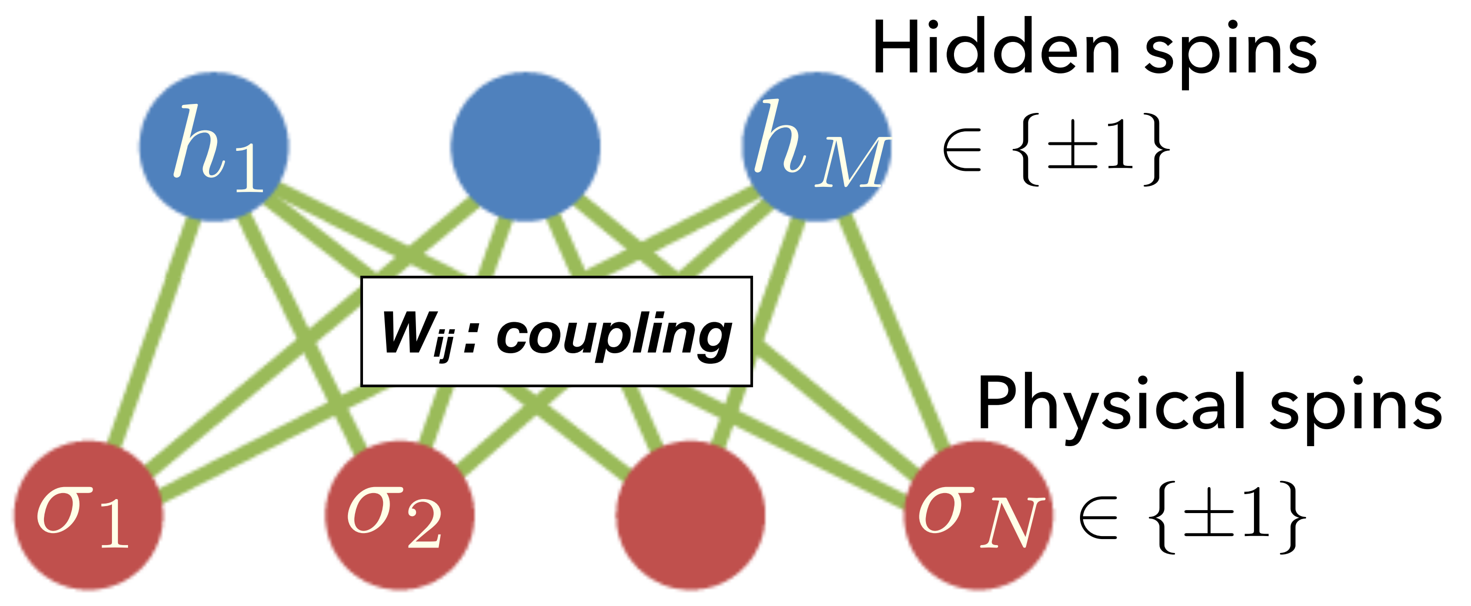
e.g. Restricted Boltzmann Machine

- Dimension-free variational ansatz inspired by machine learning
- "Universal approximator" by increasing hidden spins Roux&Bengio, Neural Comp.('08)

$$|\Psi\rangle = \sum_\sigma \Psi(\sigma)|\sigma\rangle \quad \Psi(\sigma) \propto \sum_h e^{W_{ij}\sigma_i h_j + a_i\sigma_i + b_j h_j}$$

Interaction ($W_{ij}\sigma_i h_j$), Mag. fields ($a_i\sigma_i + b_j h_j$)

h ← Tracing out aux. space



Restricted Boltzmann Machine

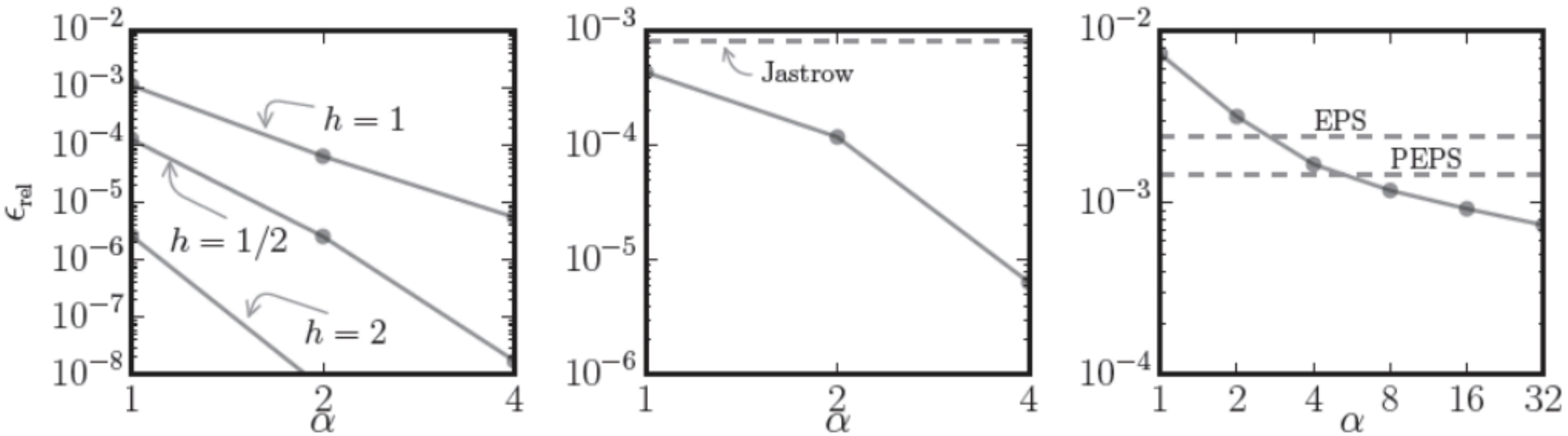
Comparison with other ansatz

State-of-art GS energy accuracy achieved by variational imaginary-time evolution

1d Traverse-field Ising model
80 spins, periodic boundary,
h : field, alpha: (# of hidden neuron)

1d AF Heisenberg model
80 spins, periodic boundary

2d AF Heisenberg model
10x10 spins, periodic boundary



Q. Are neural networks powerful enough to explore new physics?

1. Improve benchmarks quantitatively

- Advanced network structure with efficient sampling

→ **state-of-the-art in 200+qubits simulation**

Sharir et al. PRL ('20) Yang et al. NeurIPS ('20)

- Investigating quantum spin liquid under 2d frustration

Choo et al. PRB ('19) Ferrari et al. PRB ('19) Liang et al. PRB ('19) Nomura&Imada ('20)

Demonstration by deep neural net, 2d AF Heisenberg

Sharir et al. PRL ('20)

Lattice	PEPS	NAQS	QMC
10×10	-0.628601(2)	-0.628627(1)	-0.628656(2)
16×16	-0.643391(3)	-0.643448(1)	-0.643531(2)
	(tensor net)		(numerically exact)

2. Understand ansatz property

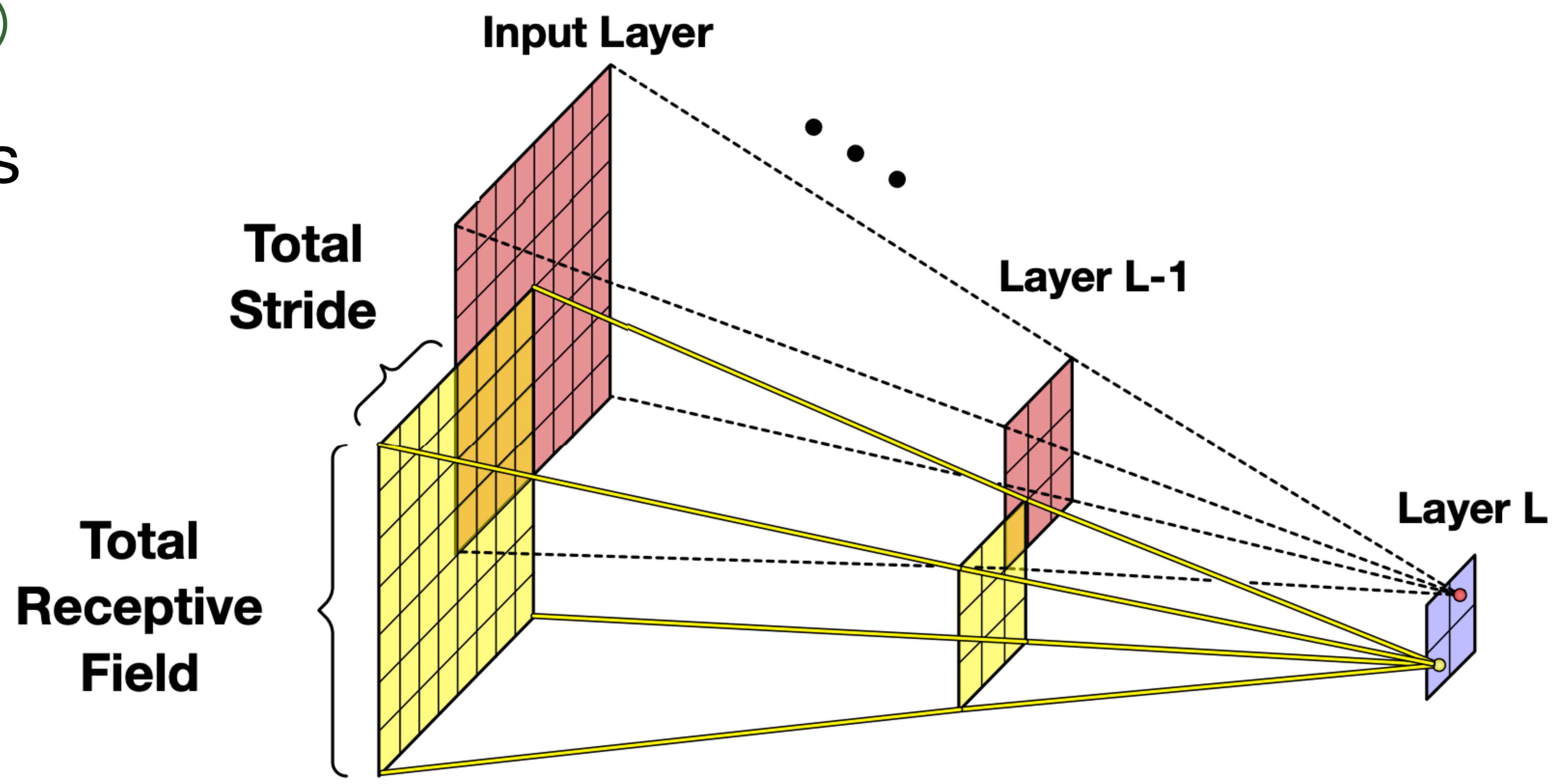
Deng et al. PRX ('17) Levine et al. PRL ('19)

- No "figure of merits" known yet for neural-net quantum states

- At least quantum entanglement is not limiting factor

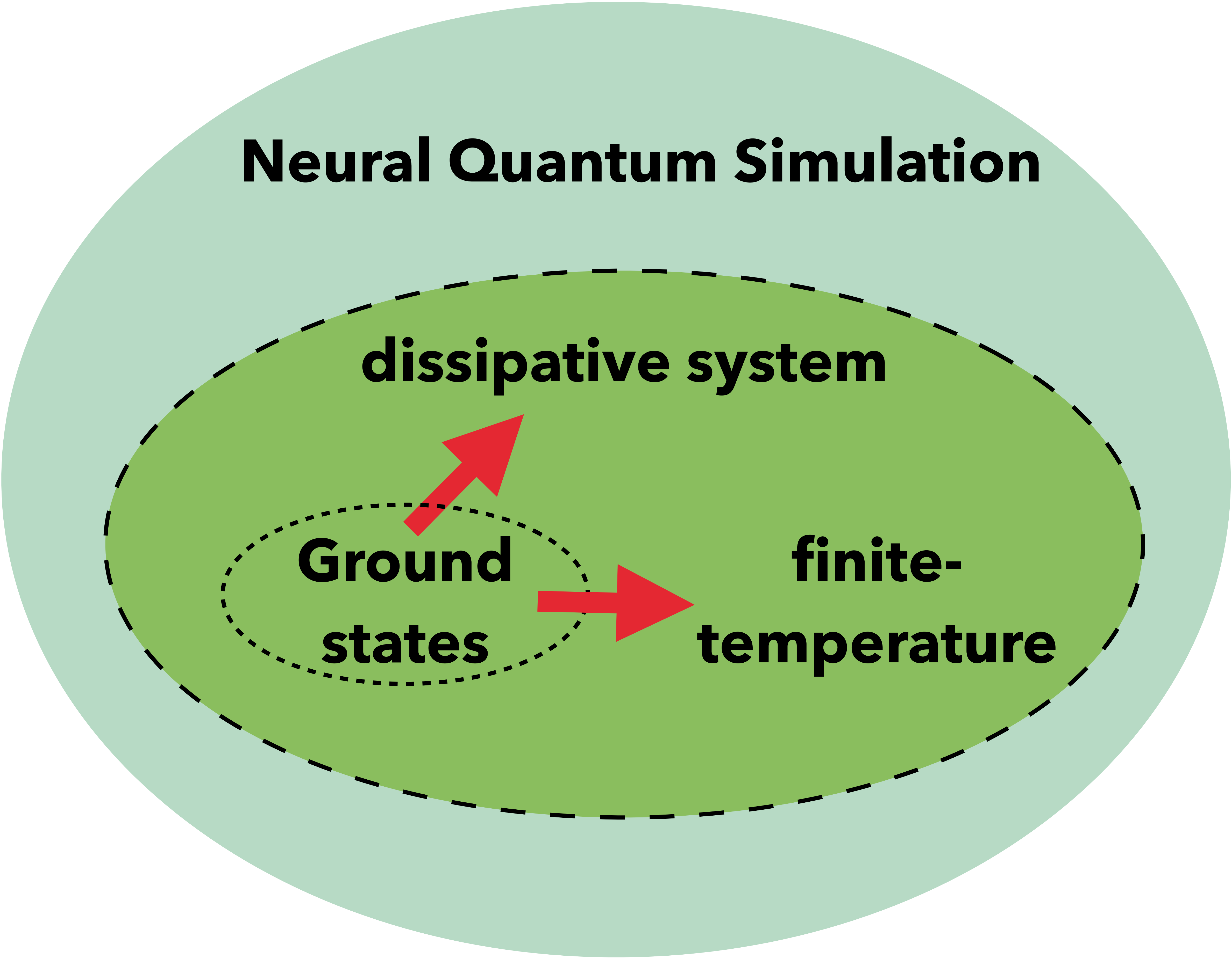
cf. #params required for volume-law ent.

- Fully-connected NN → $O(N^2)$
- RBM → $O(N)$
- Convolutional NN → $O(\sqrt{N})$



Q. Are neural networks powerful enough to explore new physics?

3. Explore algorithmically

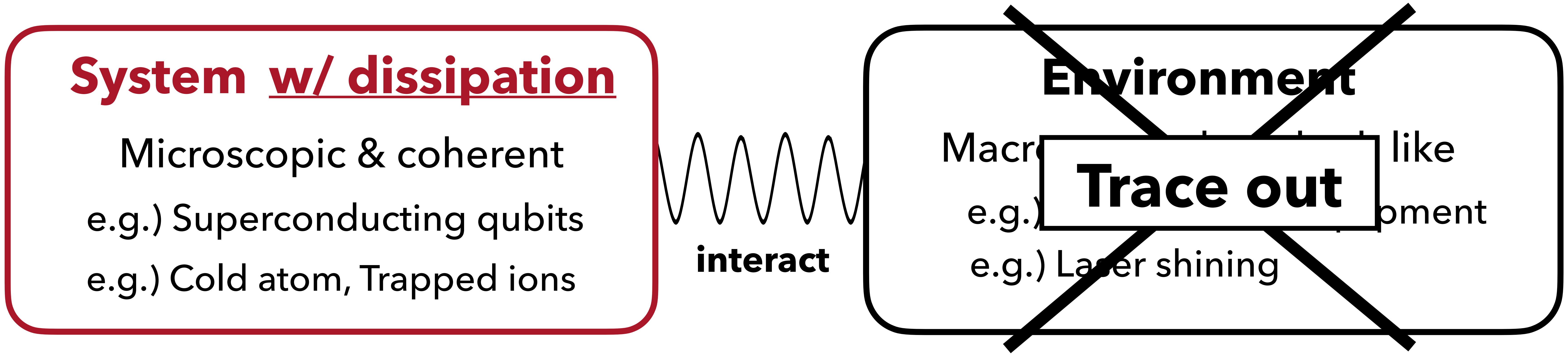


Dissipative quantum many-body problems

Why dissipative systems?

Experimental: "Realistic" physics for analyzing/pursuing highly coherent quantum devices.

Theoretical: Emergence of exotic phenomena beyond isolated quantum systems



Quantum master equation (CPTP, Markovianity imposed) Lindblad (1976) Gorini, Kossakowski&Sudarshan (1976)

- Simplest but powerful fundamental equation
- At least one <u>steady state</u> assured if time homogeneous

$$\frac{d\hat{\rho}(t)}{dt} = \mathcal{L}(t)\hat{\rho}(t) := -i[\hat{H}(t), \hat{\rho}(t)] + \mathcal{D}(t)[\hat{\rho}(t)]$$

Liouvillian; Unitary dynamics; Non-unitary, but trace-preserving

$$\mathcal{D}(t)[\hat{\rho}(t)] = \sum_s \hat{\Gamma}_s(t)\hat{\rho}(t)\hat{\Gamma}_s^\dagger(t) - \frac{1}{2}\left\{\hat{\Gamma}_s^\dagger(t)\hat{\Gamma}_s(t), \hat{\rho}(t)\right\}$$

Interests in steady states

Yoshioka&Hamazaki, Phys. Rev. B 99, 214306 (2019).

Quantum state preparation

Become “allies” with dissipation by engineering them!

- Trapping topological states in decoherence-free subspace

Kraus etal. PRA (‘08)

Verstraete etal. Nat.Phys. (‘09)

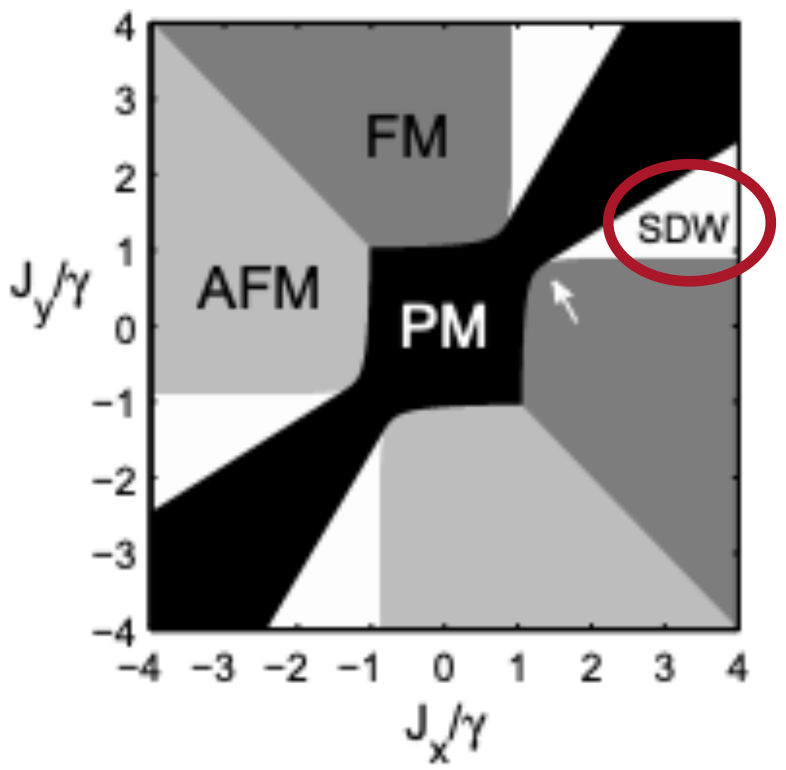
Prepare resource for universal quantum computation!

(line) $= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

(ellipse) $= |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$

Dissipation-enriched physics

- Emergence of anomalous phase

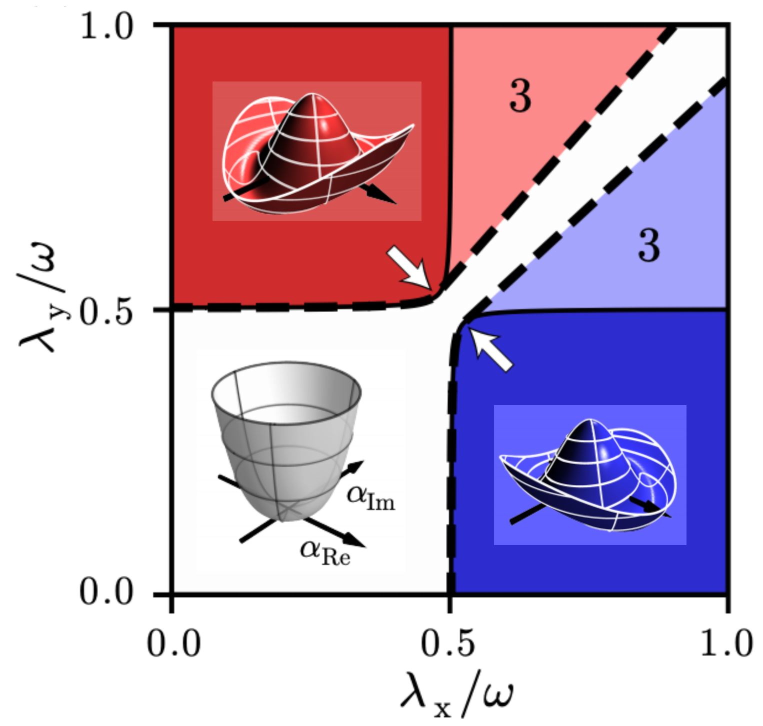


mean-field phase in XYZ+damping

Lee, Gopalakrishnan, Lukin, PRL(‘13)

- Emergence of exotic multicritical points

Soriente et al., PRL (2018)



Tricritical point with *finite* fluctuation realized with N-mode bosonic cavity

$$H = \hbar\omega_c a^\dagger a + \hbar\omega_a S_z + + \frac{2\hbar\lambda_x}{\sqrt{N}} S_x(a + a^\dagger) + \frac{2\hbar\lambda_y}{\sqrt{N}} iS_y(a - a^\dagger)$$

Variational Algorithm for Stationary states

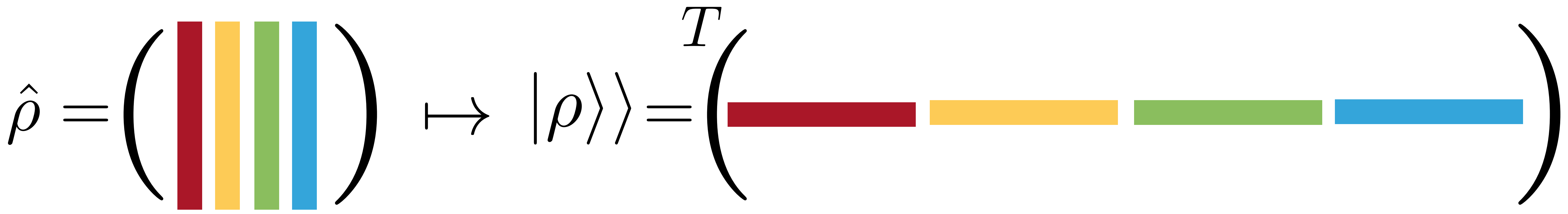
Yoshioka&Hamazaki, Phys. Rev. B 99, 214306 (2019).

Step1

Lindblad eqn. in vector representation

$$\frac{d|\rho(t)\rangle\rangle}{dt} = \hat{\mathcal{L}}|\rho(t)\rangle\rangle$$

Vector representation of density matrix



$$\hat{\rho} = \sum_{\sigma\tau} \rho_{\sigma\tau} |\sigma\rangle\langle\tau| \quad \mapsto |\rho\rangle\rangle = \frac{1}{C} \sum_{\sigma\tau} \rho_{\sigma\tau} |\sigma, \tau\rangle\rangle$$

"physical" "fictitious"

Vector representation of Lindblad equation

$$\hat{\mathcal{L}}|\rho(t)\rangle\rangle = \left(-i\left(\hat{H} \otimes \hat{1} - \hat{1} \otimes \hat{H}^T\right) + \sum_i \gamma_i \hat{\mathcal{D}}[\hat{\Gamma}_i] \right) |\rho(t)\rangle\rangle$$

non anti-hermitian

Unitary dynamics

Dissipation, Non-unitary

where $\hat{\mathcal{D}}[\hat{\Gamma}_i] = \hat{\Gamma}_i \otimes \hat{\Gamma}_i^* - \frac{1}{2}\hat{\Gamma}_i^\dagger \hat{\Gamma}_i \otimes \hat{1} - \hat{1} \otimes \frac{1}{2}\hat{\Gamma}_i^T \hat{\Gamma}_i^*$ (e.g. $\hat{\Gamma}_i = \sigma_i^-$)

Variational Algorithm for stationary states

Yoshioka&Hamazaki, Phys. Rev. B 99, 214306 (2019).

Step1

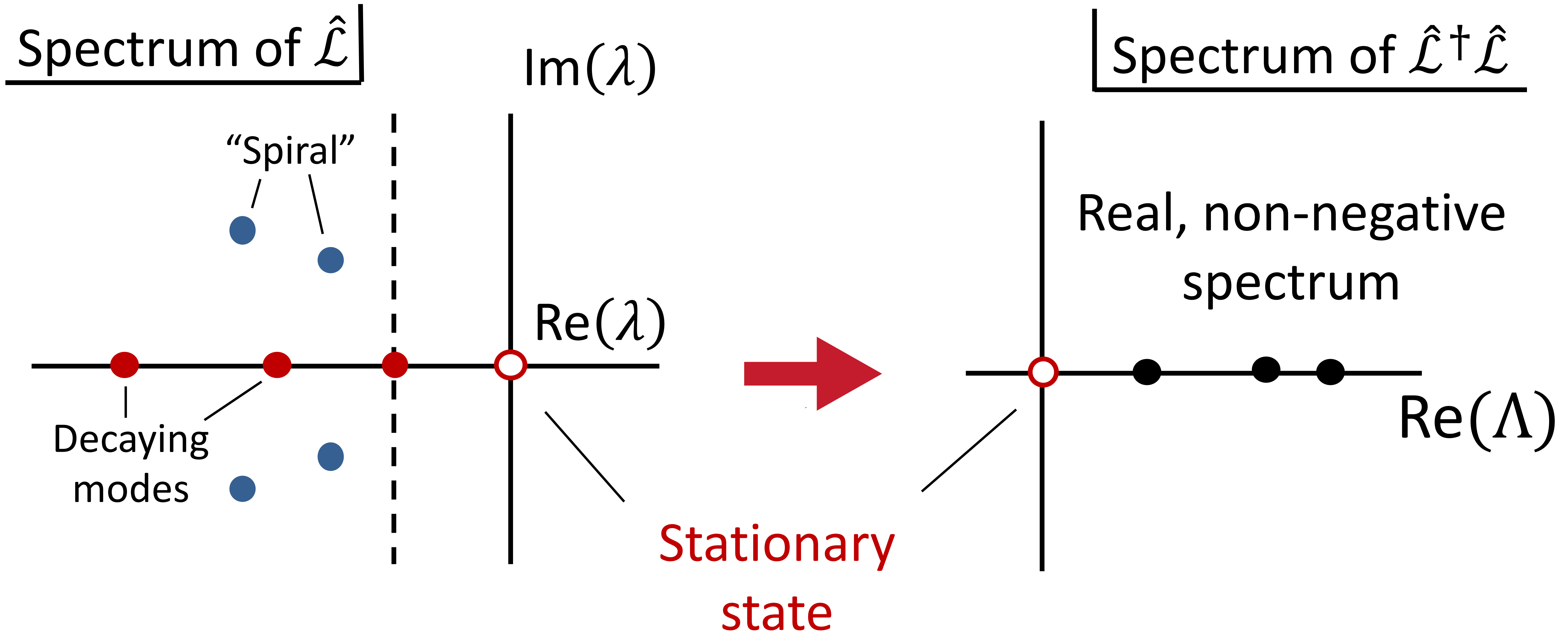
Lindblad eqn. in vector representation

$$\frac{d|\rho(t)\rangle\rangle}{dt} = \hat{\mathcal{L}}|\rho(t)\rangle\rangle$$

Step2

Define optimization task

$$\arg\min_{\rho} \frac{\langle\langle\rho|\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}|\rho\rangle\rangle}{\langle\langle\rho|\rho\rangle\rangle}$$



Steady state obtained by

$$0 = \underset{\rho}{\mathrm{argmin}} \frac{\langle\langle\rho|\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}|\rho\rangle\rangle}{\langle\langle\rho|\rho\rangle\rangle}$$

Our goal

Cui etal. PRL ('15)

Variational Algorithm for stationary states

Yoshioka&Hamazaki, Phys. Rev. B 99, 214306 (2019).

Step1

Lindblad eqn. in vector representation

$$\frac{d|\rho(t)\rangle\rangle}{dt} = \hat{\mathcal{L}}|\rho(t)\rangle\rangle$$

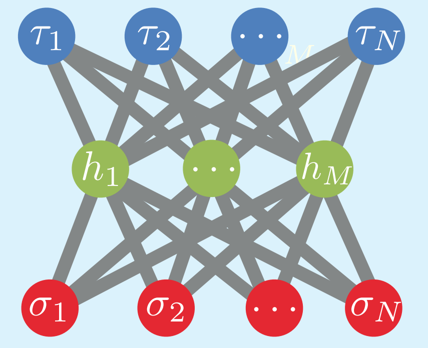
Step2

Define optimization task

$$\arg\min_{\rho} \frac{\langle\langle\rho|\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}|\rho\rangle\rangle}{\langle\langle\rho|\rho\rangle\rangle}$$

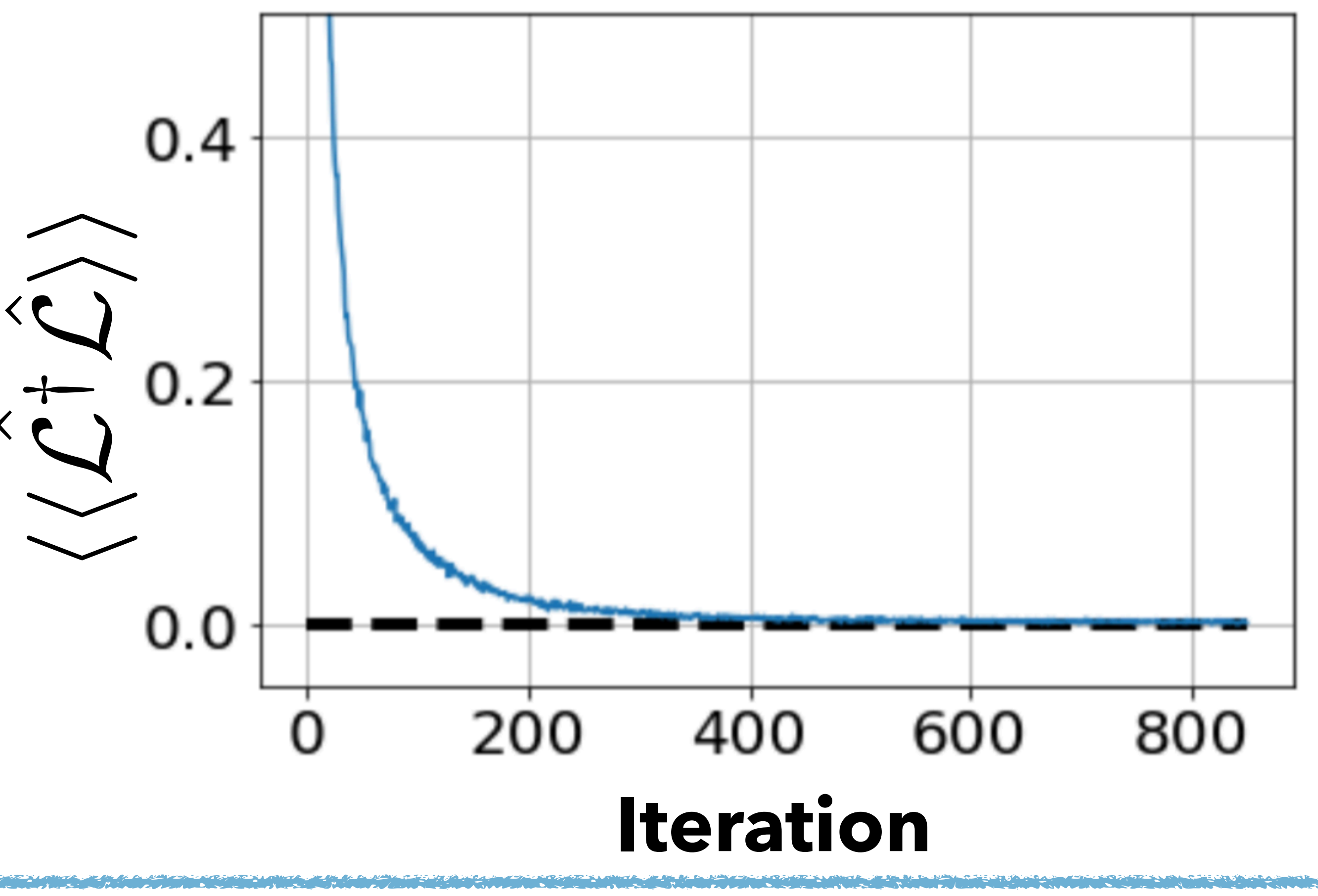
Step3

Ansatz selection

$$|\rho\rangle\rangle = \Big|$$  $$\Big\rangle\Big\rangle$$

Step4

Run optimization



Precisely zero if exact

Demonstrations

Yoshioka&Hamazaki, Phys. Rev. B 99, 214306 (2019).

<u>e.g. Transverse-field Ising model w/ damping</u> Barreior etal. Nature ('11) Carr etal. PRL ('13)

Realized in trapped ions, Rydberg atoms

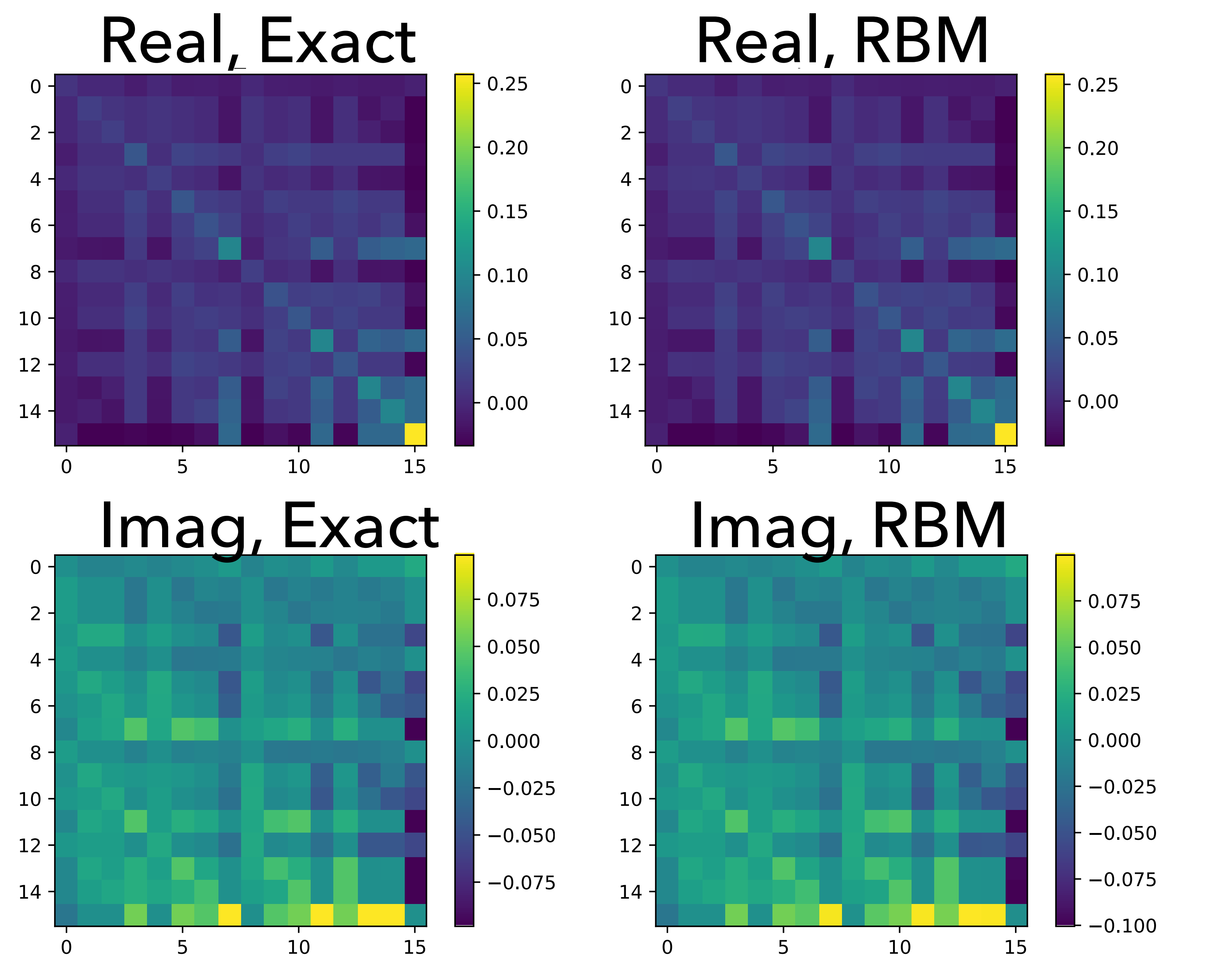
$$\hat{H} = \frac{V}{4}\sum_{i=0}^{L-1}\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z + \frac{g}{2}\sum_{i=0}^{L-1}\hat{\sigma}_i^x, \text{ with } \hat{\Gamma}_i = \hat{\sigma}_i^-,$$

<u>1d TFIM with damping</u>

- Fidelity > 0.995 achieved up to L=16 (32 spins) at g/V = 0.3
- 40-fold #parameter reduction at strong field compared to MPS (L=16, reported by Hartmann&Carleo)

<u>2d TFIM with damping</u> Jin etal. PRB ('18)

- Fidelity > 0.999 achieved for 2x2, 3x3 at g/V = 1
- Cost function optimized (~10^{-3}) up to 5x5



Real/Imaginary part of density matrices
2d TFIM, V=1, g=1, γ=1, fidelity>0.999

Demonstration done, to be applied to explore new physics!

Finite-temperature problems

Nomura, Yoshioka, Nori, arXiv:2103.04971

Why finite-temperature?

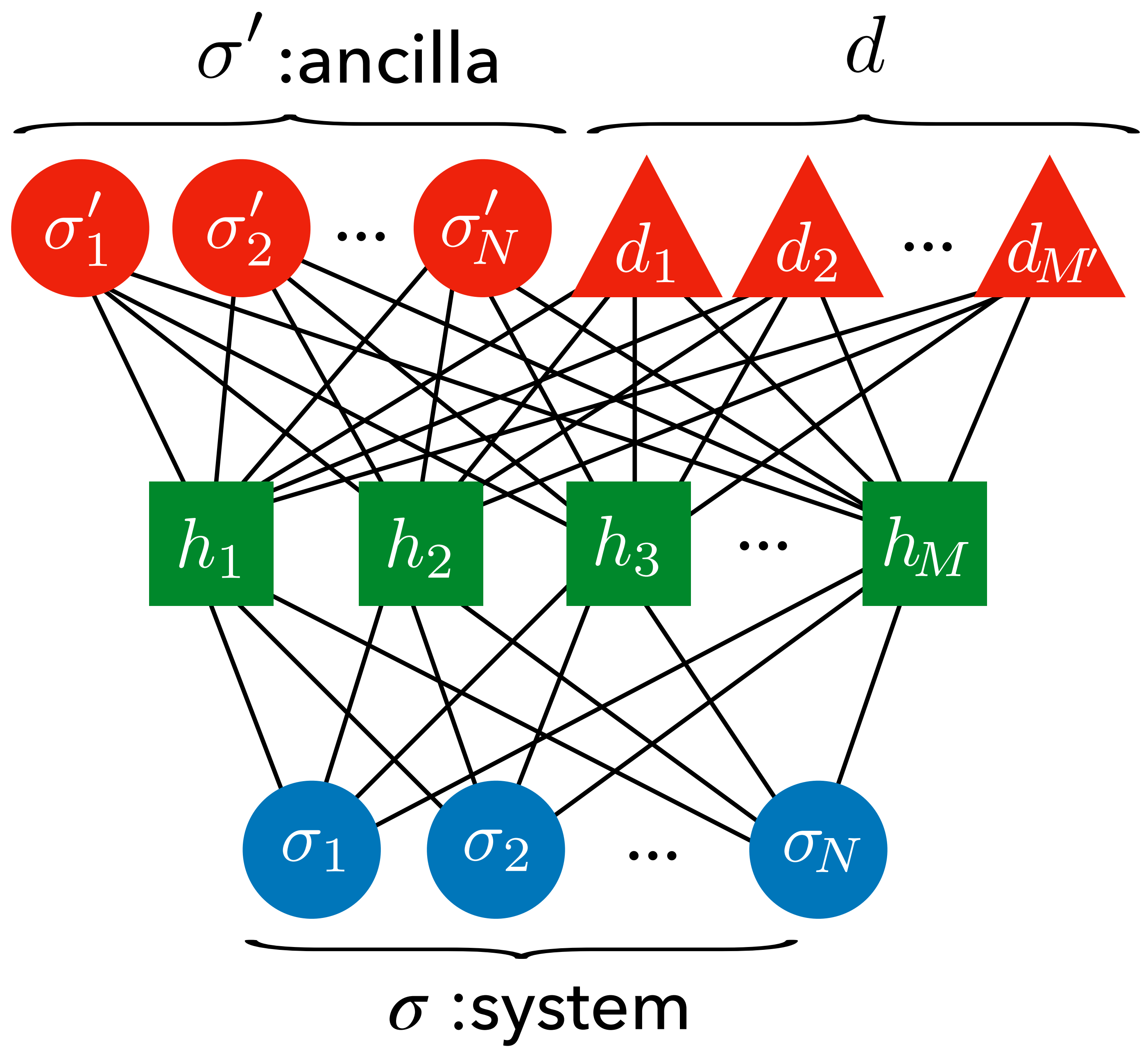
- Most important regime to be challenged: frustration, strongly-correlated electrons in 2D etc.
  - tensor-networks → focused on 1D for T>0 so far
  - DMFT → accuracy in large coordination-numbers, not necessarily ideal for 2D

Our neural-network-based algorithms

Main idea: Purifying Gibbs state ρ using Deep Boltzmann machine

$$\rho = \frac{1}{Z} e^{-\beta H} = \mathrm{Tr}_{\mathscr{A}}[\,|\Psi_T^{(\mathrm{DBM})}\rangle\langle\Psi_T^{(\mathrm{DBM})}|\,]$$

$$= \frac{1}{Z}\mathrm{Tr}_{\mathscr{A}}[e^{-\beta H/2}|\Psi_{T=\infty}^{(\mathrm{DBM})}\rangle\langle\Psi_{T=\infty}^{(\mathrm{DBM})}|e^{-\beta H/2}]$$



Method (I) : Exact representation of purified Gibbs states

Method (II) : Approximate imaginary-time evolution

Method (I): Exact Gibbs DBM

Nomura, Yoshioka, Nori, arXiv:2103.04971

DBM representation of Suzuki-Trotter decomposition

- By splitting the Hamiltonian as $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$, the purified state written as

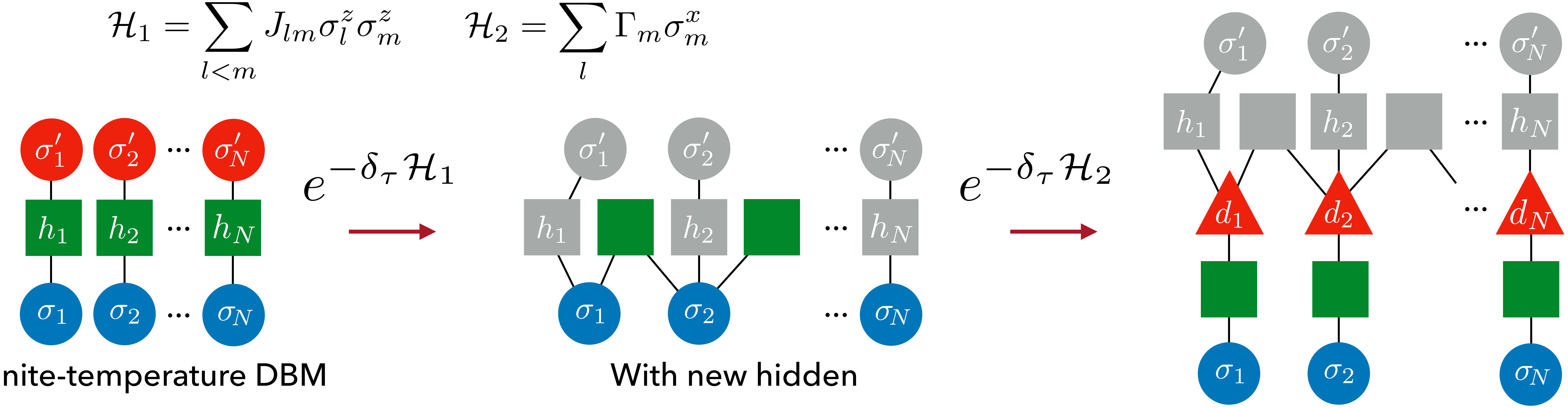
$$|\Psi_T\rangle := \left(\left[e^{-\delta_\tau \mathcal{H}_2} e^{-\delta_\tau \mathcal{H}_1} \right]^{N_\tau} \otimes \mathbb{I}' \right) |\Psi_{T=\infty}\rangle, \quad \text{where } |\Psi_{T=\infty}\rangle = \bigotimes_i \frac{(|\uparrow\downarrow'\rangle - |\downarrow\uparrow'\rangle)}{\sqrt{2}}$$

- We find exact representation of purified states at arbitrary T by finding

$$|\Psi'_{\mathrm{DBM}}\rangle \propto e^{-\delta_\tau \mathcal{H}_\nu} |\Psi_{\mathrm{DBM}}\rangle$$

<u>e.g. Transverse-field Ising model</u>

$$\mathcal{H}_1 = \sum_{l<m} J_{lm} \sigma_l^z \sigma_m^z \qquad \mathcal{H}_2 = \sum_l \Gamma_m \sigma_m^x$$



Method (I): Exact Gibbs DBM

Nomura, Yoshioka, Nori, arXiv:2103.04971

DBM representation of Suzuki-Trotter decomposition

- By splitting the Hamiltonian as $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$, the purified state written as

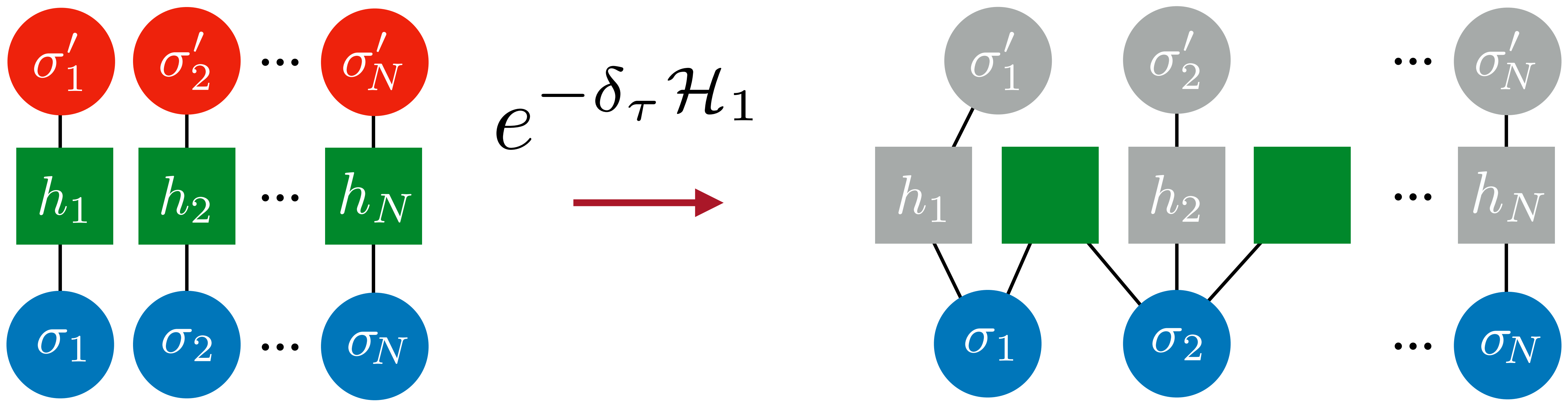
$$|\Psi(T)\rangle := \left(\left[e^{-\delta_\tau \mathcal{H}_2} e^{-\delta_\tau \mathcal{H}_1} \right]^{N_\tau} \otimes \mathbb{I}' \right) |\Psi(T{=}\infty)\rangle,$$

- We find exact representation of purified states at arbitrary T by finding

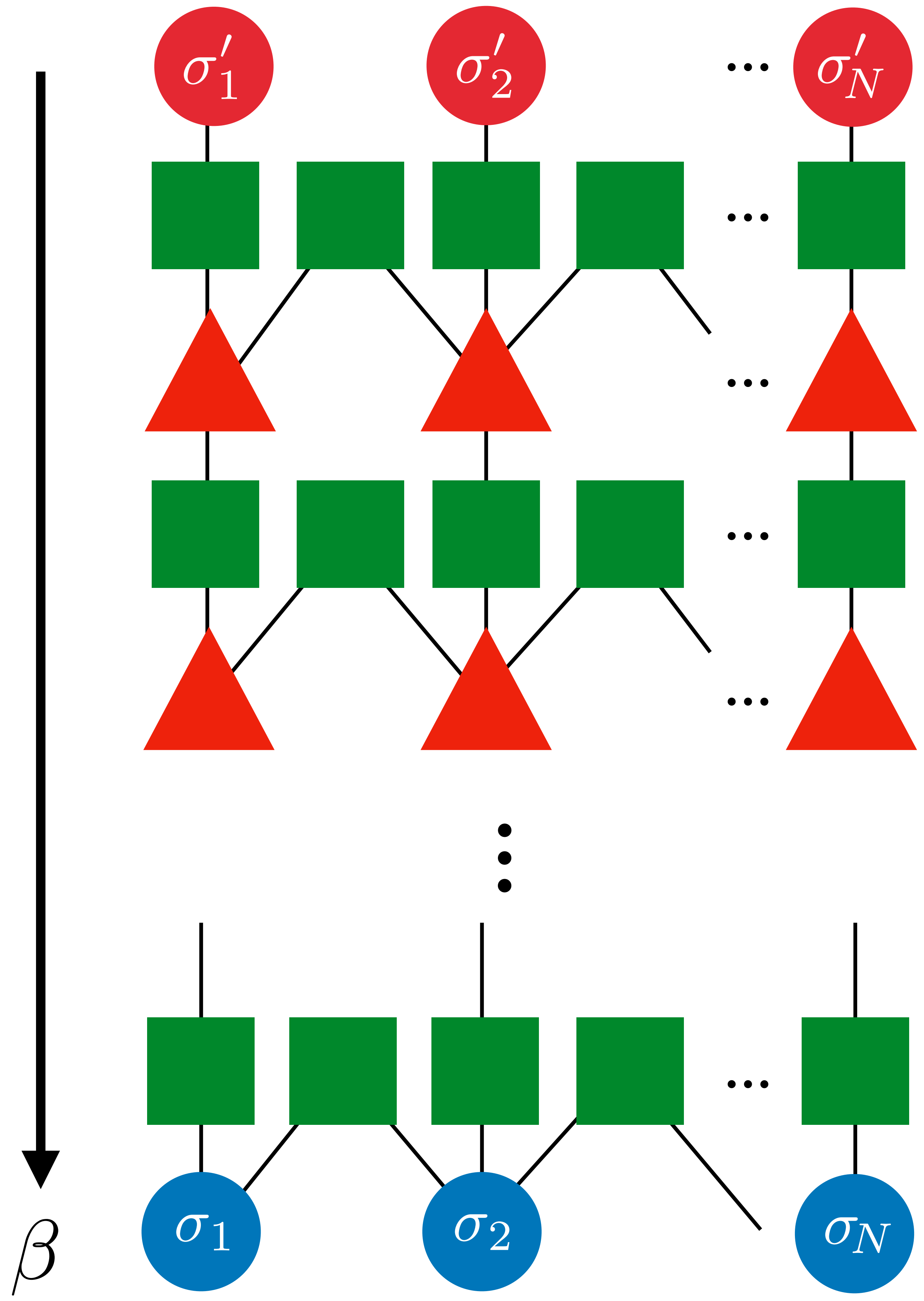
$$|\Psi'_{\mathrm{DBM}}\rangle \propto e^{-\delta_\tau \mathcal{H}_\nu} |\Psi_{\mathrm{DBM}}\rangle$$

e.g. Transverse-field Ising (TFI) model

$$\mathcal{H}_1 = \sum_{l<m} J_{lm} \sigma_l^z \sigma_m^z \qquad \mathcal{H}_2 = \sum_l \Gamma_m \sigma_m^x$$



Infinite-temperature DBM   With new hidden



Method (I): Exact Gibbs DBM

Nomura, Yoshioka, Nori, arXiv:2103.04971

DBM representation of Suzuki-Trotter decomposition

- By splitting the Hamiltonian as $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$, the purified state written as

$$|\Psi(T)\rangle := \left(\left[e^{-\delta_\tau \mathcal{H}_2} e^{-\delta_\tau \mathcal{H}_1} \right]^{N_\tau} \otimes \mathbb{I}' \right) |\Psi(T = \infty)\rangle,$$

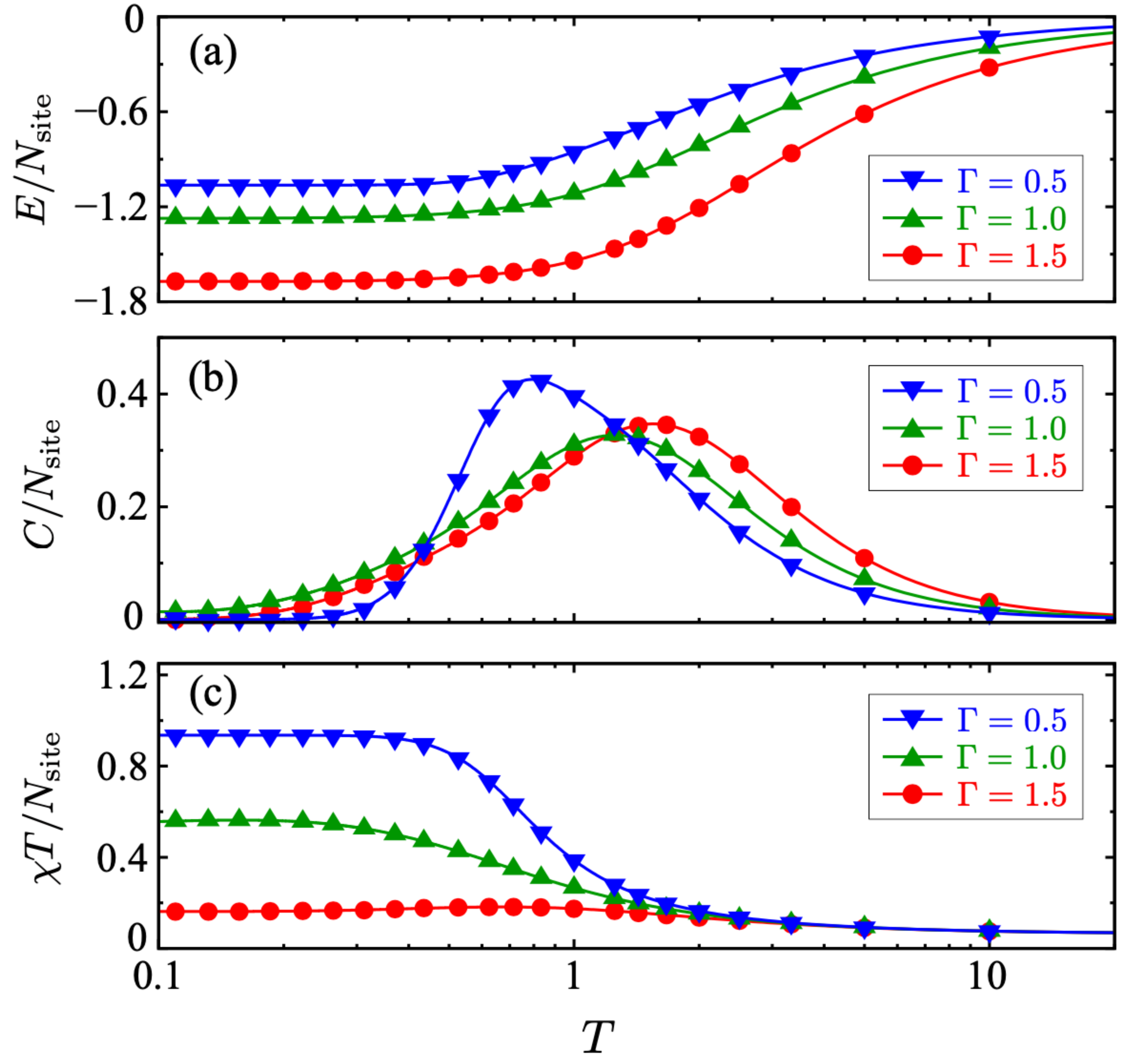
- We find exact representation of purified states at arbitrary T by finding

$$|\Psi'_{\mathrm{DBM}}\rangle \propto e^{-\delta_\tau \mathcal{H}_\nu} |\Psi_{\mathrm{DBM}}\rangle$$

e.g. Transverse-field Ising (TFI) model

$$\mathcal{H}_1 = \sum_{l<m} J_{lm} \sigma_l^z \sigma_m^z \qquad \mathcal{H}_2 = \sum_l \Gamma_m \sigma_m^x$$

DBM-based calculation for 1d TFI (16 sites)



Path-integral formalism for certain class of Hamiltonian completely mapped into DBM

Method (II): Approximate Gibbs DBM

Nomura, Yoshioka, Nori, arXiv:2103.04971

Use of variational principle

- In the presence of negative-signs, we employ **stochastic reconfiguration**:

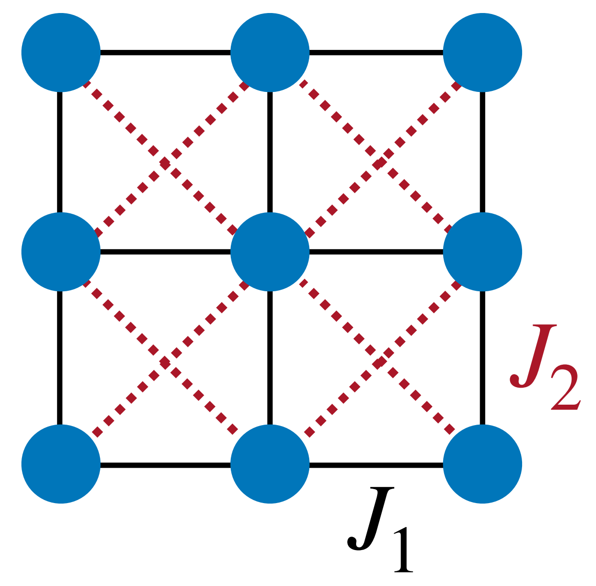
$$\underbrace{\delta\mathcal{W}}_{\text{network parameter}} = \arg\min_{\delta\mathcal{W}} \left(\mathcal{F}\left(\underbrace{e^{-\delta_\tau \mathcal{H}}|\Psi_{\mathcal{W}}\rangle}_{\text{exact evol.}}, \underbrace{|\Psi_{\mathcal{W}+\delta\mathcal{W}}\rangle}_{\text{approx. evol.}}\right)\right)$$

$\mathcal{F}$: Fubini-Study metric

$$= i\delta_\tau \underline{S^{-1}}\, \underline{\partial_{\mathcal{W}}\langle\mathcal{H}\rangle}$$

S : Quantum Fisher info.

evaluated by MC



Demonstration in 2d J1J2 Heisenberg model (square lattice)

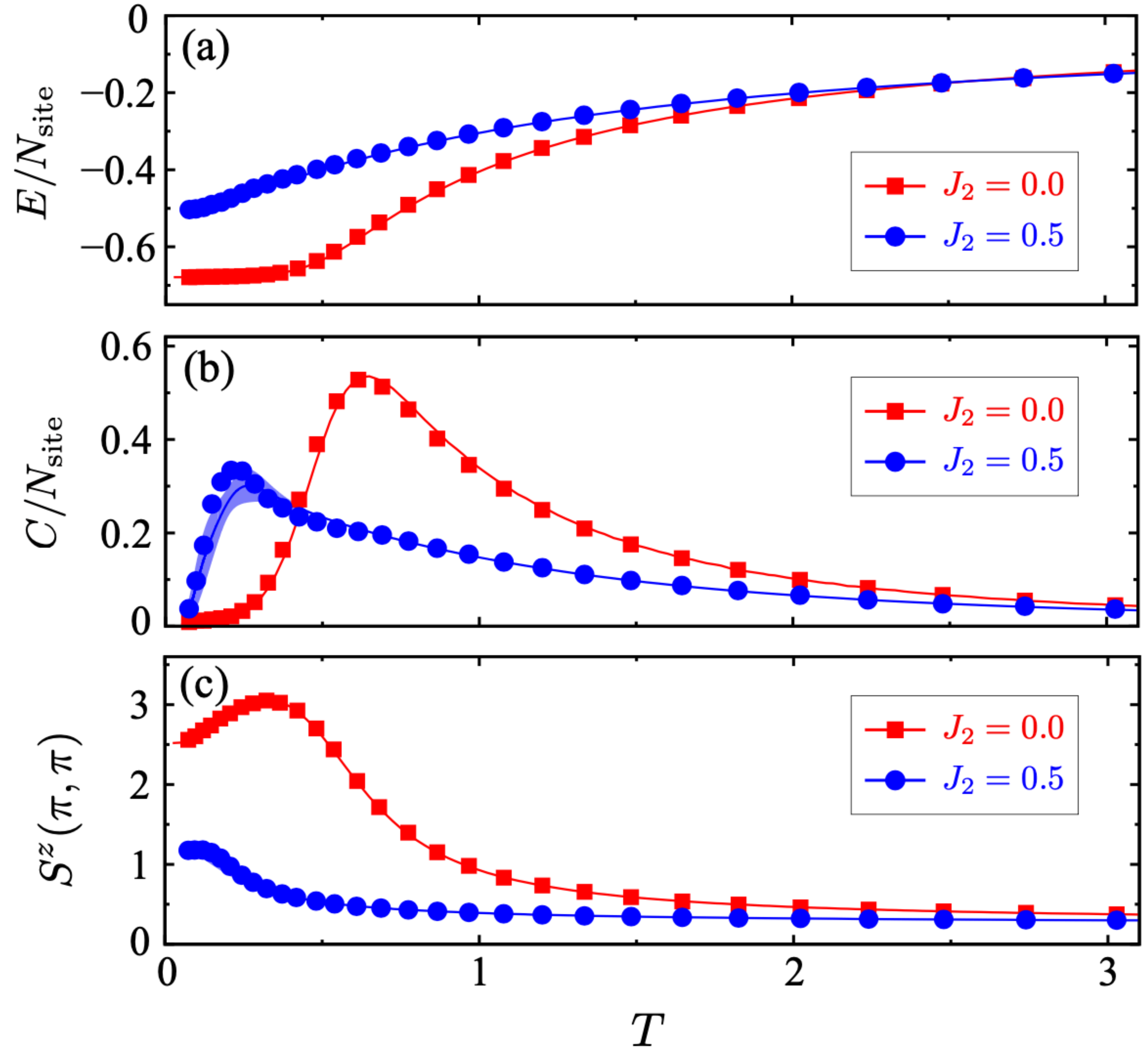
- Excellent match with TPQ (J2=0.5) , also with QMC at J2=0

- $O(N_h N^2)$ observed as computational scaling

  where N:#sites, N_h : (#hidden spins)

- Strongly advancing NN-calculations for exploring exotic physics

2d J1-J2 Heisenberg (6x6 sites, total Sz=0)



Summary

Solving dissipative quantum many-body system by shallow NN

NY & R. Hamazaki, PRB 99, 214306 (2019).

- Vectorized density matrix encoded in RBM
- Steady-state search as zero-eigenvalue problem tested up to 5x5 sites
- Extension to non-Markovian, search for dissipation-induced exotic phase, quantum trajectory…

Finite-temperature calculation by Deep NN

Nomura, **NY**, Nori, arXiv:2103.04971

- Purified Gibbs states encoded in DBM
- Exact representation using quantum-to-classical mapping
  Approximate representation useful even under negative signs
- Intensive search for quantum spin liquid phase under finite T?