Quantum many-body dynamics from neural networks with GPU acceleration

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1. Introduction

Solving quantum-mechanical problems is, in general, exponentially hard in the number of degrees of freedom N

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

Quantum state — Complex amplitudes — Computational basis (e.g. spin configurations)

Key problem: full information requires storage of all amplitudes

Exponential growth of Hilbert space: $\#s \propto e^{CN}$

Number of amplitudes grows generally exponentially

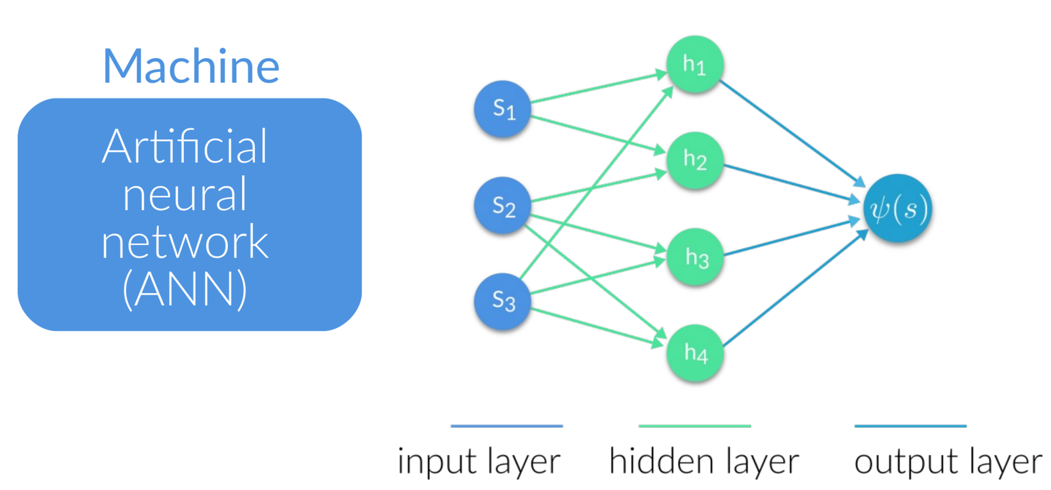
Possible solutions:
- efficient compression
- reduction to effective simplified descriptions
- ...

Challenge: No known (numerically exact) solution for **nonequilibrium** states in **two and three spatial dimensions**

2. Encoding quantum states in neural networks

Idea: "Don't store, generate on the fly"

- Sample from machine using Monte-Carlo techniques
- Avoids storage of amplitudes



Enabling idea: ANNs **universal function approximators**

- Any quantum state can be encoded in a (sufficiently large) ANN

Complexity of algorithm: poly(size of ANN, #DOF)

Carleo & Troyer, Science '17

Where's the problem then? Training....

Schmitt & Heyl, arXiv: 1912.08828

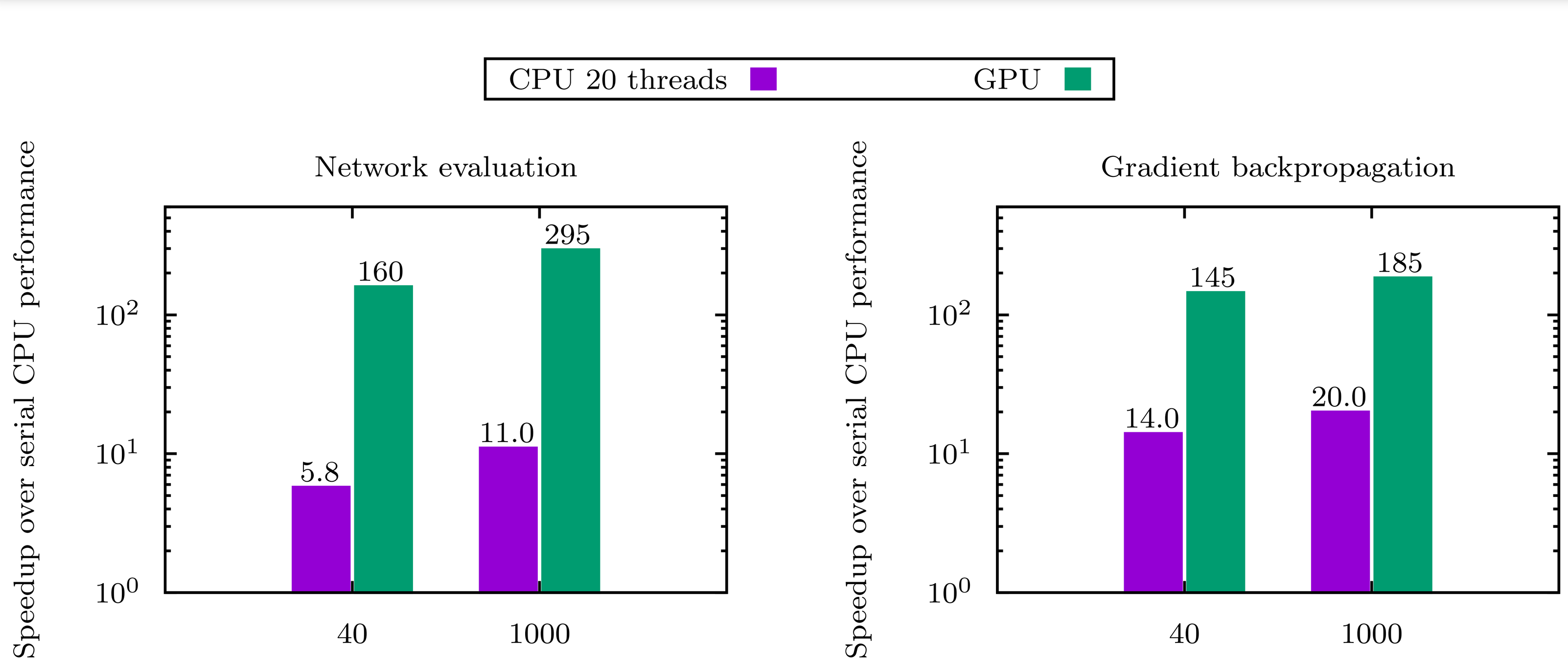
Quantum real-time evolution: time-dependent variational principle

Variational Monte-Carlo with ANN as variational wave function

3. Parallel implementation

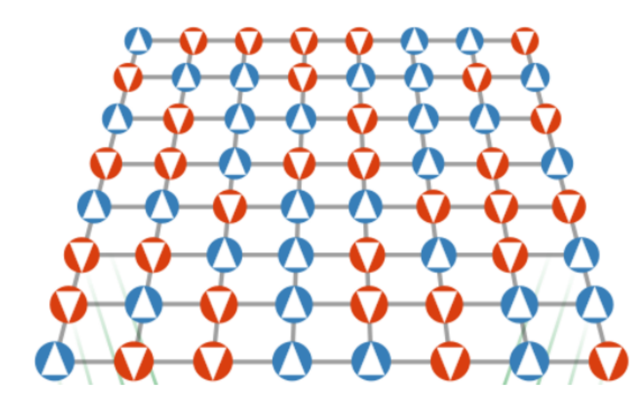
Multiple levels of parallelism:

- Monte-Carlo (trivially parallel) ⟶ MPI (multiple nodes)
- Network evaluation ⟶ CUDA (for GPUs)



3. Quantum dynamics in 2D

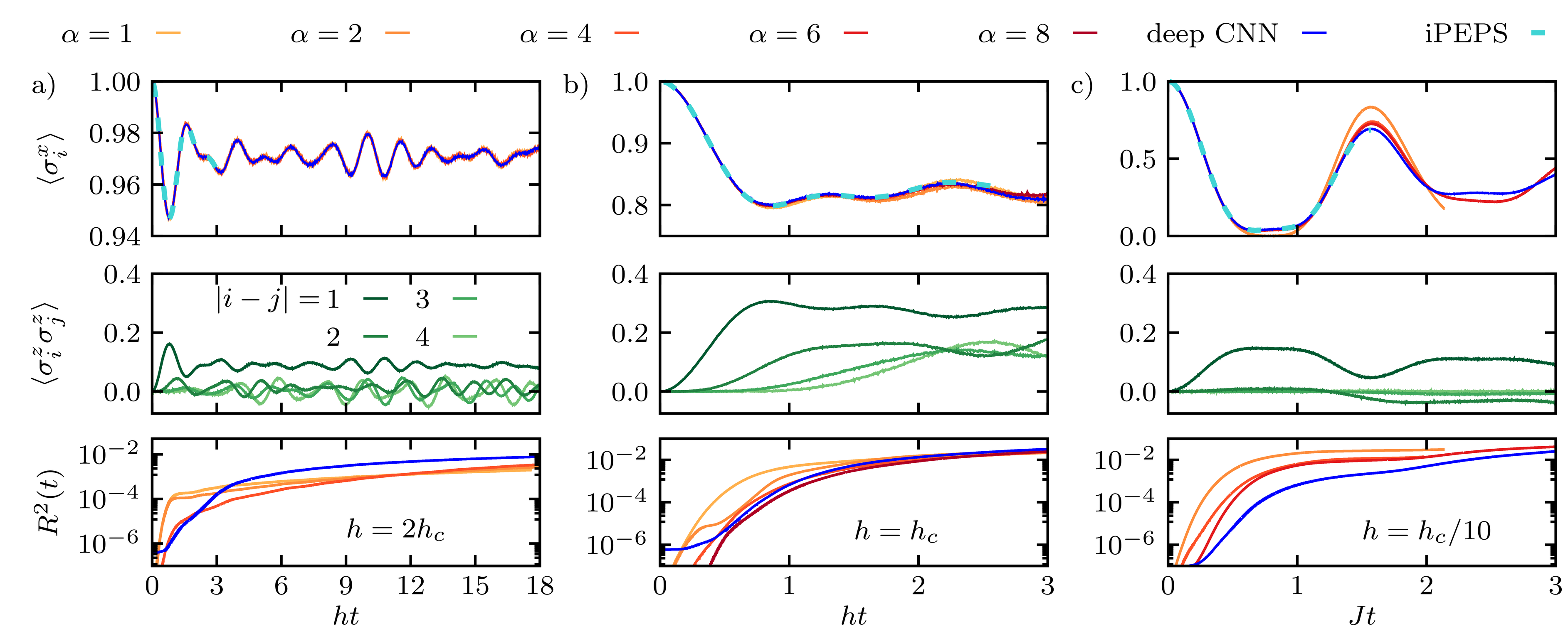
Schmitt & Heyl, arXiv: 1912.08828



Transverse-field Ising model on a square lattice

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

Quantum quench: initial condition $|\psi_0\rangle = |\rightarrow\rangle$



Agreement with iPEPS up to reached time scales

iPEPS: numerically exact, longer times very hard

Main limitation: training & instabilities, not expressivity!

4. Quantum renormalization groups

- Fully many-body localized (MBL) systems: emergent constants of motion τ_i:

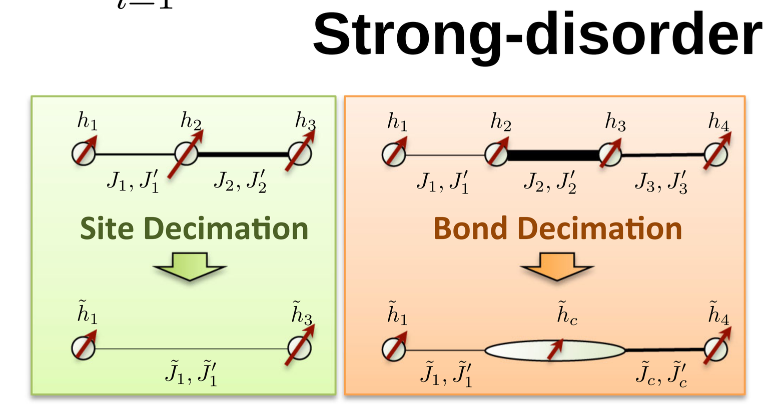
$$\tilde{H} = T^\dagger H T = \sum_i \alpha_i\tau_i + \sum_{ij}\beta_{ij}\tau_i\tau_j + \ldots \qquad T\text{: local unitary}$$

- **Idea:** use a quantum renormalization group (RG) transformation to obtain T.
- **Goal:** Describe non-equilibrium long-time dynamics in MBL systems.

Model: Non-integrable, disordered quantum Ising chain

$$H = \sum_{i=1}^{L} J_i\,\sigma_i^z\sigma_{i+1}^z + K_i\,\sigma_i^x\sigma_{i+1}^x + h_i\,\sigma_i^x,\quad J_i\in[0,J], K_i\in[0,0.1\cdot J], h_i\in[0,h]$$

Strong-disorder renormalization group



[1]

$$\tilde{H} = e^{-iS}He^{iS} = \prod_m e^{-iS_m} H \prod_m e^{iS_m}$$

Schrieffer-Wolff (SW) transformation

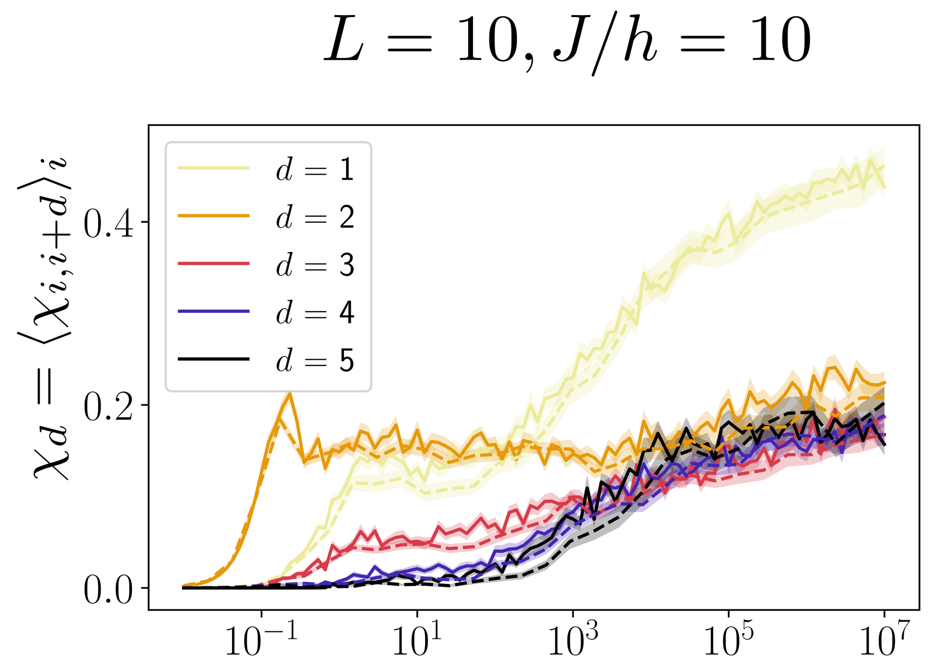
BUT: Taking into account the SW unitary for the calculation of observables is challenging ⟶ **encode the unitary in an artificial neural network (ANN).**

Idea: unitary transformation = time evolution

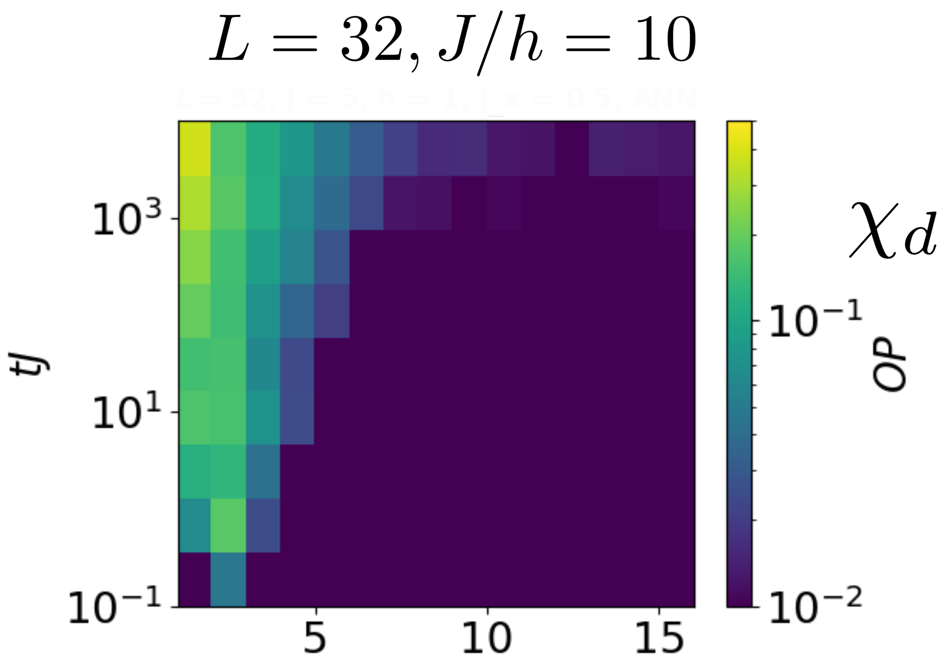
Thus: use same formalism as before

- **Quantum quench:** Time evolution starting from $|\psi_0\rangle = |\rightarrow\rangle$
- MBL-spin glass order parameter: $\chi_{i,j=i+d} = \sum_{n=1}^{4} p_n^{ij}\,\langle\psi_n^{ij}|\sigma_i^z\sigma_j^z|\psi_n^{ij}\rangle^2$

eigenvalues, eigenstates of reduced two-site density matrix



Comparison to exact diagonalization (dashed: RG + ANN, solid: ED)



Slow (logarithmic) buildup of long-range order