LMC2 – Simulating nonequilibrium quantum many-body systems with neural quantum states

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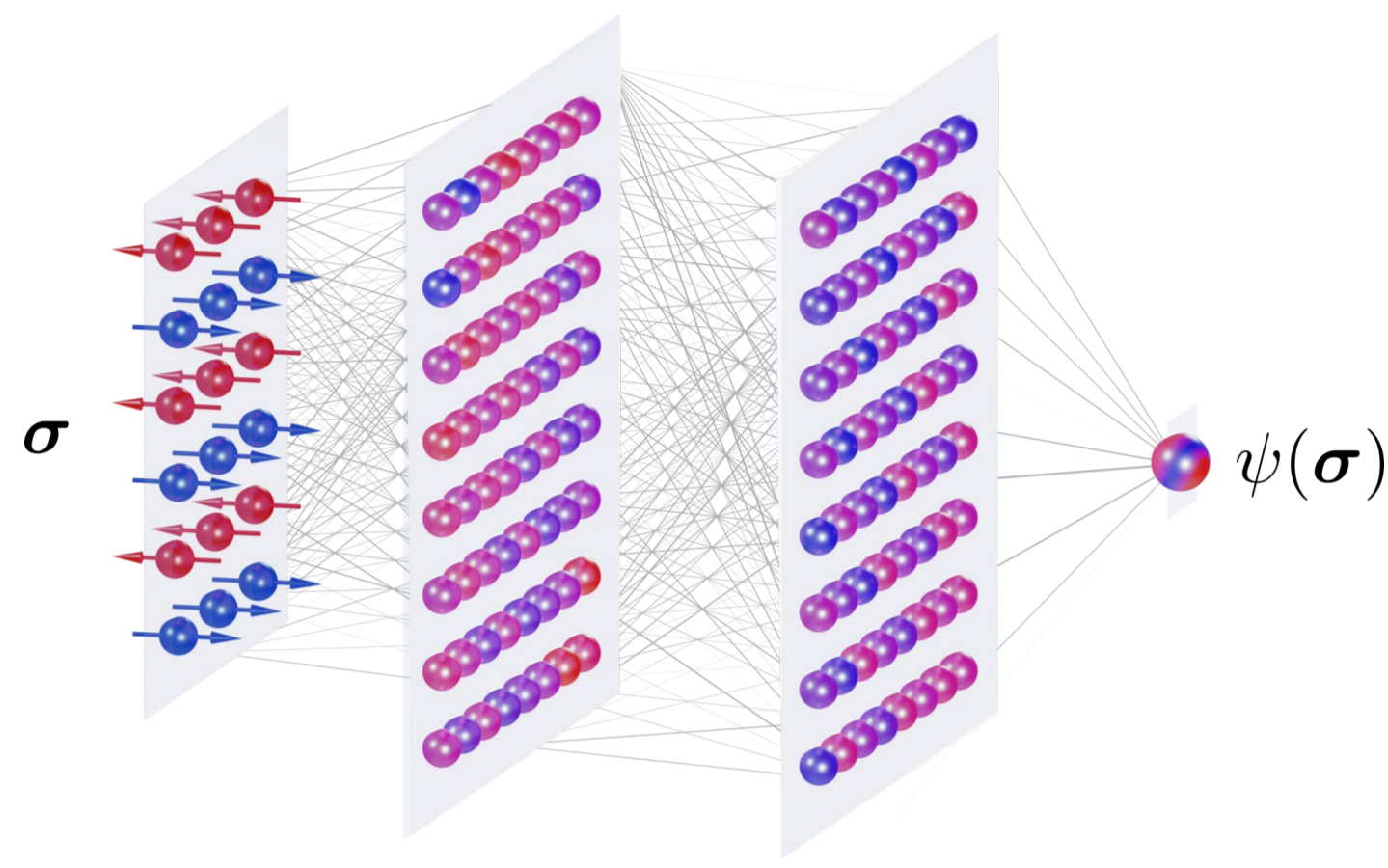
Introduction

Figure 1: Illustration of a neural quantum state for a two-dimensional spin system. The neural network is used to represent the mapping from a spin configuration to its corresponding probability amplitude.
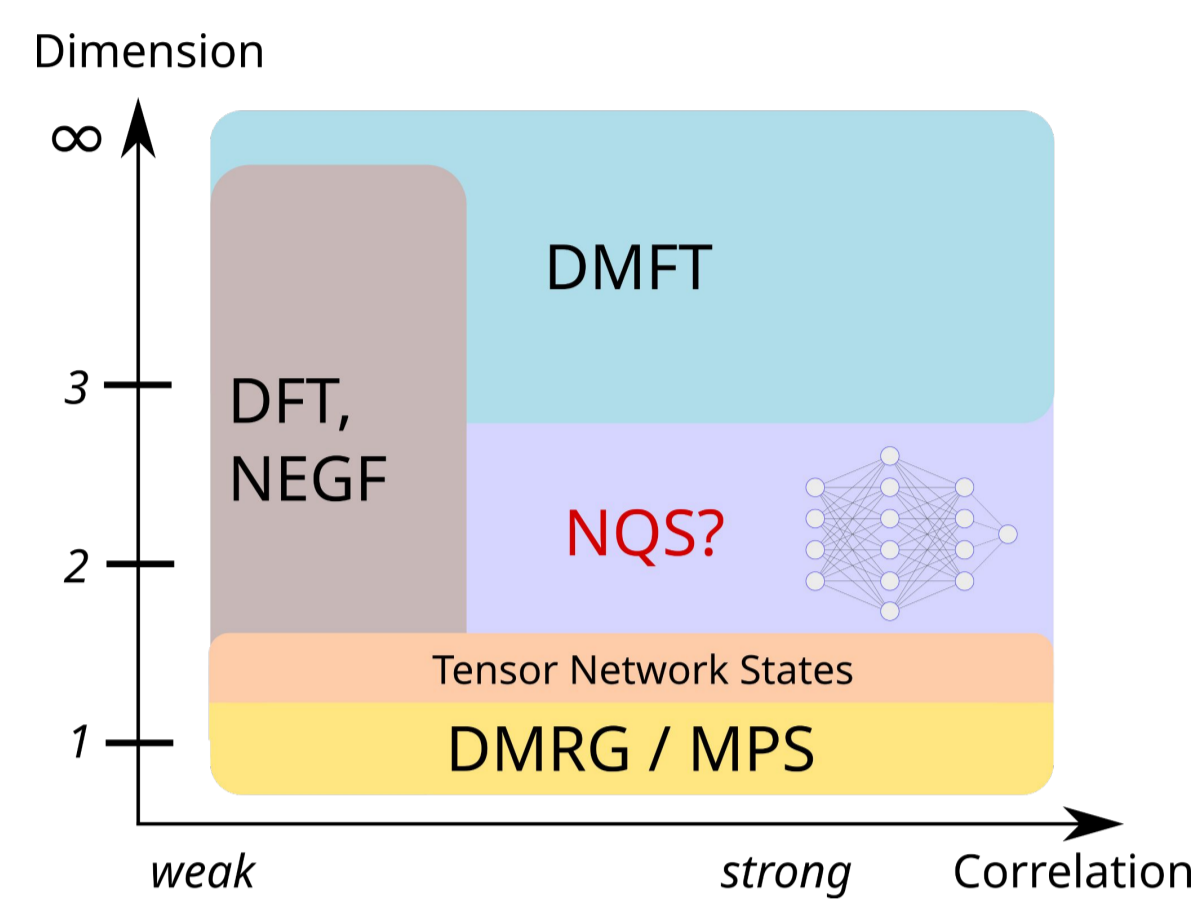

Figure 2: NQS have shown some potential to fill an important gap in the current lineup of computational methods for simulating strongly correlated two-dimensional systems.

In recent times, machine-learning inspired methods have started to play an increasingly important role in many areas of physics. Among those methods are neural quantum states (NQS), which are a class of variational states for which the mapping from basis configuration to probability amplitudes of a trial state is expressed by a neural network. The network weights are trained as variational parameters (Fig. 1).

NQS are not constrained by volume-law entanglement scaling and have been successfully used to simulate dynamical properties of two-dimensional Heisenberg and Ising model systems (Fig. 2). Here, we present results and currently ongoing projects of our own work on utilizing NQS for studying dynamics in such systems.

Stability of NQS time propagation algorithms

In collaboration with Giammarco Fabiani, Johan H. Mentink (Radboud University) and Giuseppe Carleo (EPFL).

- In NQS methods, quantum expectation values of observables and their gradients are approximated by variational Monte Carlo (VMC), i.e., by "classical" stochastic sampling over the Born distribution $|\psi(\boldsymbol{\sigma})|^2$.

- Neural quantum states can be time-propagated using time-dependent variational Monte Carlo (t-VMC), which is based on a stochastic approximation of the time-dependent variational principle (TDVP).

$$\delta\theta = \arg\max_{\delta\eta} |\langle e^{-i\delta t\hat{H}}\psi_\theta|\psi_{\theta+\delta\eta}\rangle|^2 \quad\Leftrightarrow\quad \sum_j \underbrace{\left[\langle\partial_i\psi_\theta|1-\hat{P}_{|\psi_\theta\rangle}|\partial_j\psi_\theta\rangle\right]}_{\text{Quantum Fisher matrix (QFM)}} \dot\theta_j = -i\underbrace{\langle\partial_i\psi_\theta|\hat{H}|\psi_\theta\rangle}_{\text{Energy gradient}}$$

t-VMC equation of motion

- The stability of this propagation method has been identified as a key challenge in several works, whereas the representation capabilities of the ansatz were not a limiting factor.

- In our project, we have performed a systematic analysis of stability properties and sources of error in small benchmark system [1], comparing the antiferromagnetic Heisenberg model on a square lattice versus a two-leg ladder.
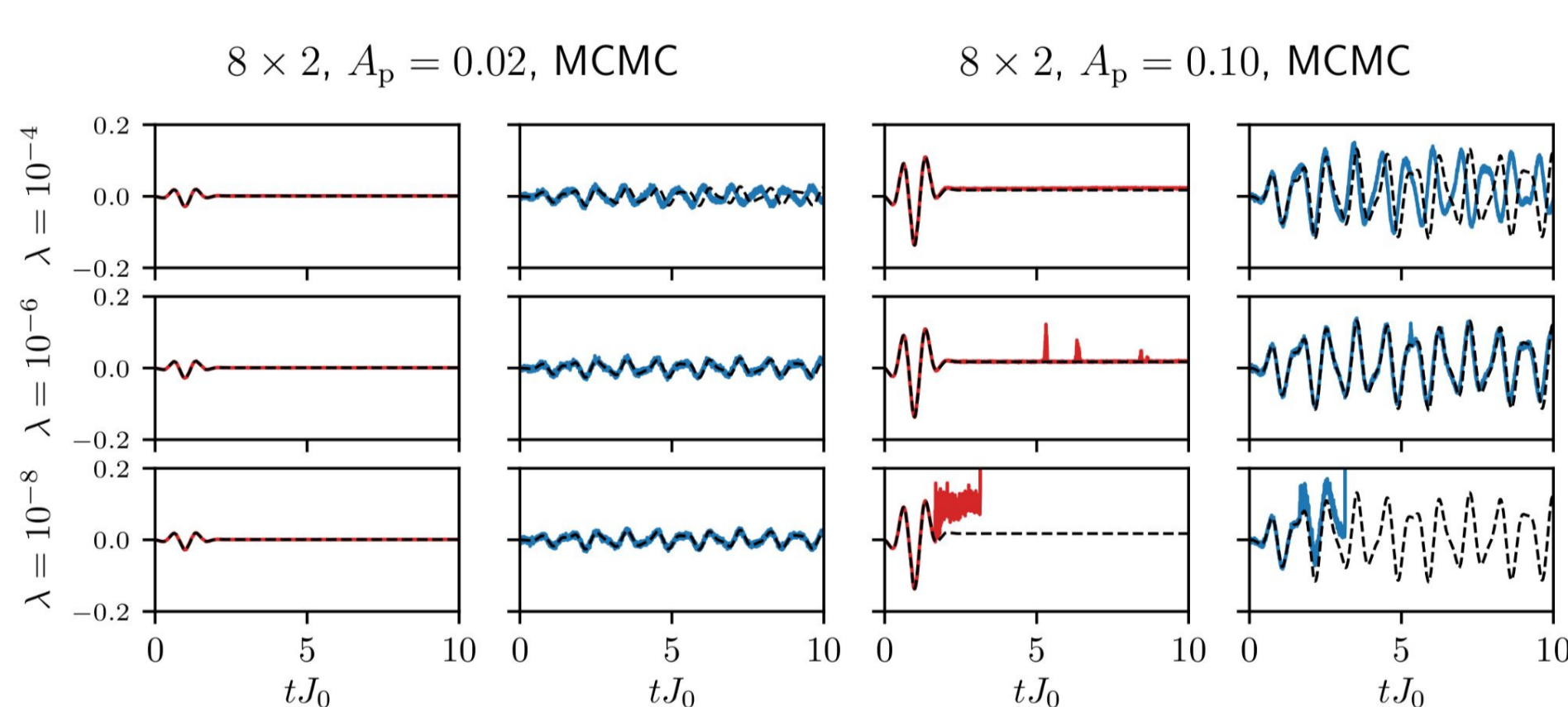

Figure 3: Numerical instabilities in t-VMC propagation can occur, depending on regularization strength λ. Stability improves with increased regularization, but physical dynamics are suppressed when the regularization becomes too strong.
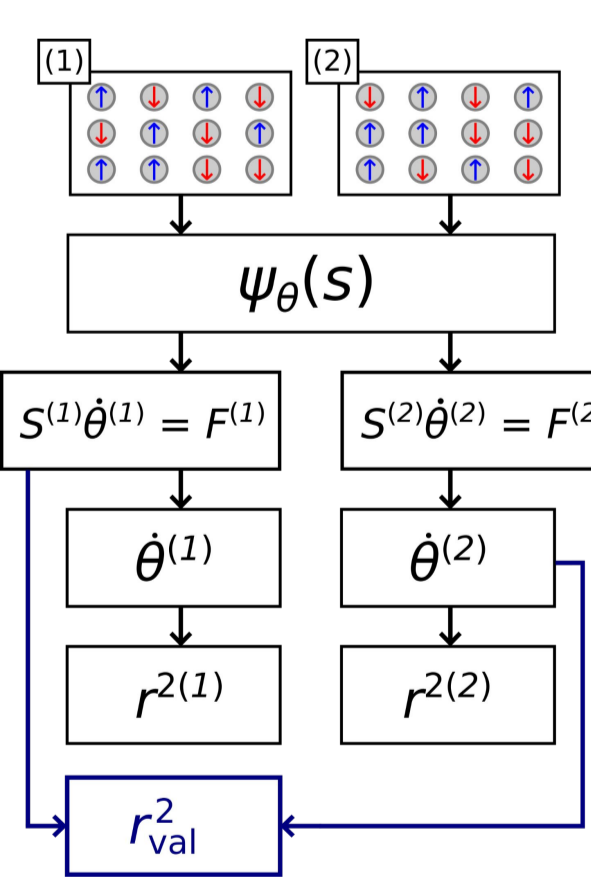

Figure 4: Validation error for assessing the consistency of parameter gradients.

- Unmitigated noise is strongly amplified by the nonlinear equation of motion, which causes numerical instability in the propagation. Regularization is required to remedy these instabilities, which however comes at the cost of accuracy in the overregularized regime (Fig. 3).

- We provide an interpretation of instabilities as caused by overfitting to a specific realization of the noisy equation of motion and propose a validation-set error diagnostic inspired by ML practice to assist with tuning hyperparameters for a stable and accurate propagation (Fig. 4).

- We expect that implementing and improving this and other types of diagnostics and regularization schemes will be an important step towards reliable and widely usable NQS time propagation algorithms.

NetKet – Machine learning toolkit for quantum physics

In collaboration with Giuseppe Carleo and Filippo Vicentini (EPFL) as well as many other NetKet contributors.

- NetKet is a software framework providing machine learning models and methods for quantum physics built around neural quantum states and variational Monte Carlo algorithms [2, 3].

- NetKet is developed as a collaborative open source project with contributors from several research institutions. Our own code is built on NetKet and in the interest of growing the NQS community and software ecosystem, we contribute back improvements and new features to the project.

- Key features of the current version (NetKet 3) include the ability to define networks in pure Python (supporting just-in-time compilation and automatic differentiation through the JAX framework), comprehensive support for discrete symmetry groups, and built-in support for t-VMC propagation.

www.netket.org

Learning quantum spin liquid phases of matter

In collaboration with Martin Claassen (University of Pennsylvania).

- The two-dimensional antiferromagnetic Heisenberg model on the square lattice was among the first systems successfully simulated with NQS methods. Recent advances in network architectures have made it possible to efficiently learn states with more complex sign structures.

- In this project we apply symmetric NQS based on group-convolutional neural networks (GCNNs) to a generalization of the Kitaev-Heisenberg model (Fig. 5), with the aim of studying the nonequilibrium physics of α-RuCl$_3$.
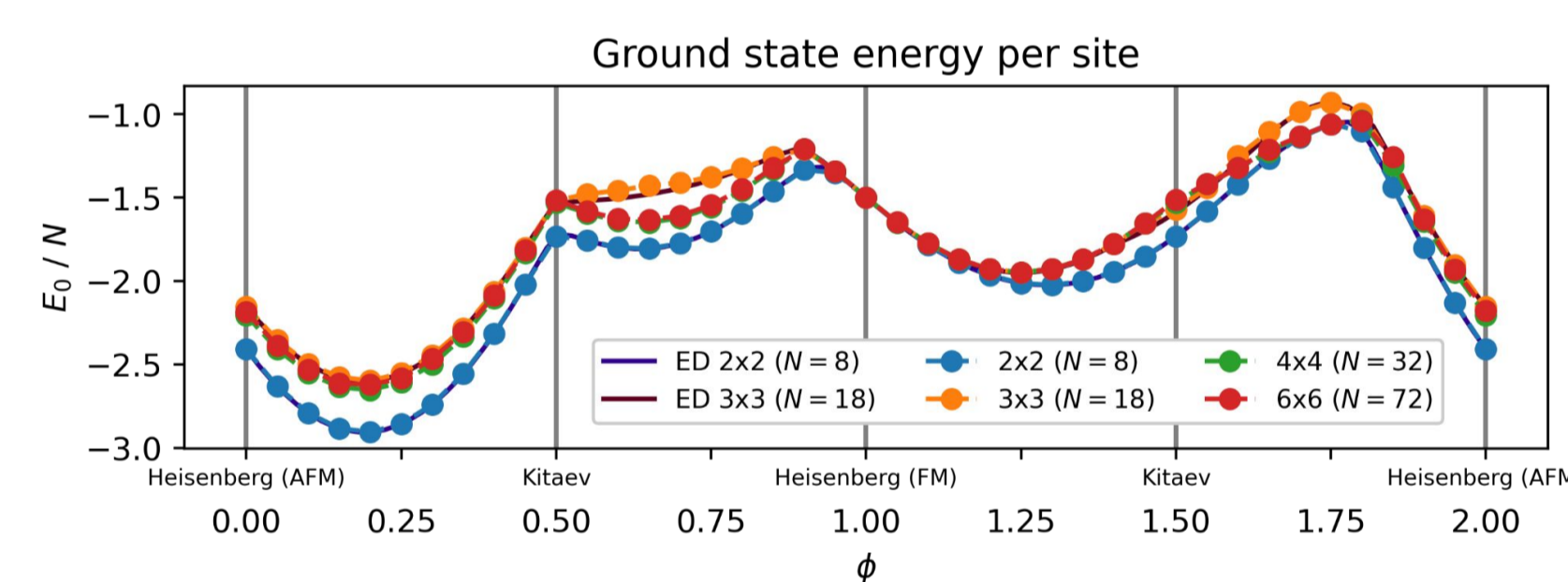

Figure 5: Optimized variational ground state energy using a GCNN ansatz for varying system sizes up to 6×6 unit cells with 72 sites. The mixing parameter ϕ determines the relative strength of Kitaev and Heisenberg interactions.

Representative capabilities of NQS for the SYK model

In collaboration with Giacomo Passetti (RWTH Aachen).

- The abilities of NQS to represent and learn specific quantum states are important questions of current research.

- In this ongoing project, we study the Sachdev-Ye-Kitaev (SYK) and random-hopping model (RHM). Both models feature volume-law entanglement, making them ideal candidates to investigate NQS capabilities.

- In our first results (Fig. 6), we observe that NQS can learn the ground state of specific realizations of the SYK model in small systems. We compare results for a multi-layer feed-forward network (FFNN) to the restricted Boltzmann machine (RBM).

$$\hat{H} = \sum_{ij} t_{ij}\hat{c}_i^\dagger\hat{c}_j \qquad \text{RHM}$$
$$\mathbb{E}[t_{ij}^* t_{pq}] = \frac{1}{N}\delta_{ip}\delta_{jq}$$

$$\hat{H} = \sum_{ijkl} J_{ijkl}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_l\hat{c}_k \qquad \text{SYK}$$
$$\mathbb{E}[J_{ijkl}^* J_{pqrs}] = \frac{1}{N^2}\delta_{ip}\delta_{jq}\delta_{kr}\delta_{ls}$$
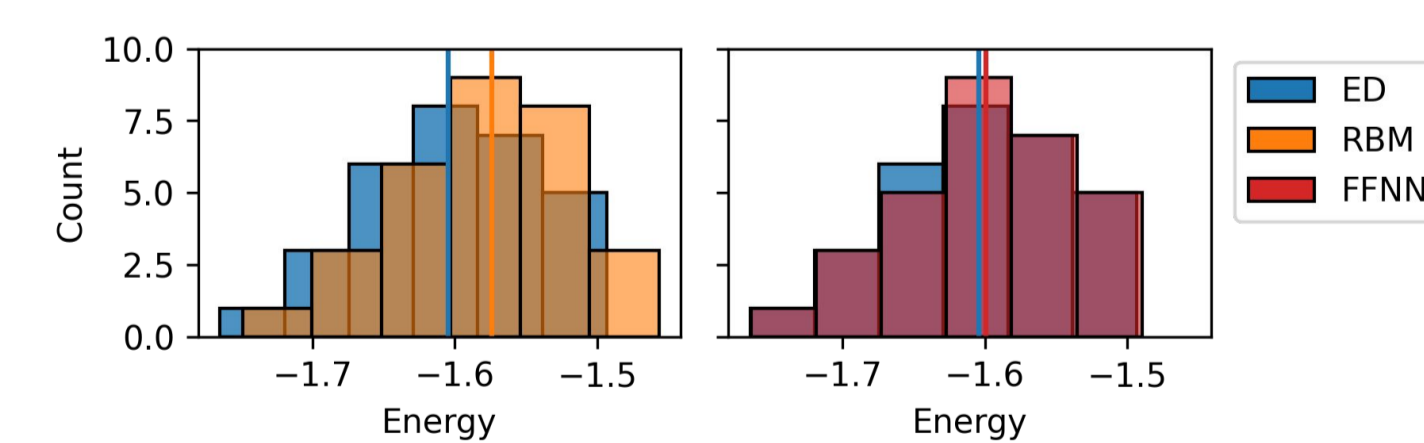

Figure 6: Ground state energy distributions for the 12-site SYK model for two neural network architectures compared with ED data.

Conclusion

We have presented our work on the development of widely usable open source software for NQS computations, improving algorithms for time propagation, and our ongoing efforts on applying NQS to quantum spin liquids as well as understanding which properties determine whether a quantum state is learnable by an NQS.

References

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[3] Vicentini, DH, Szabó, Wu, Roth et al., arXiv:2112.10526