Title: Leveraging recurrence in neural network wavefunctions for large-scale simulations of Heisenberg antiferromagnets

Speakers: Megan Schuyler Moss

Collection/Series: Training Programs (TEOSP)

Subject: Other

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Abstract:

Machine-learning-based variational Monte Carlo simulations are a promising approach for targeting quantum many-body ground states, especially in two dimensions and in cases where the ground state is known to have a non-trivial sign structure. While many state-of-the-art variational energies have been reached with these methods for finite-size systems, little work has been done to use these results to extract information about the target state in the thermodynamic limit. In this work, we employ recurrent neural networks (RNNs) as a variational ansätze, and leverage their recurrent nature to simulate the ground states of progressively larger systems through iterative retraining. This transfer learning technique allows us to simulate spin-1/2 systems on very large lattices without beginning optimization from scratch for each system size, thus reducing the demands for computational resources. We first examine the square-lattice Heisenberg antiferromagnet, where it is possible to carefully benchmark our results. We also study the more challenging, sign-problematic triangular-lattice Heisenberg antiferromagnet. In both cases, we show that we are able to systematically improve the accuracy of our simulations by increasing the training time. Furthermore, we use our finite-size results to extract accurate estimates of ground-state properties in the thermodynamic limit. These works demonstrate that RNN wavefunctions are able to extract accurate information about quantum many-body systems in the thermodynamic limit.

Leveraging recurrence in neural network wavefunctions for large-scale simulations of Heisenberg antiferromagnets

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Grad Student Seminar
Dec 1, 2025

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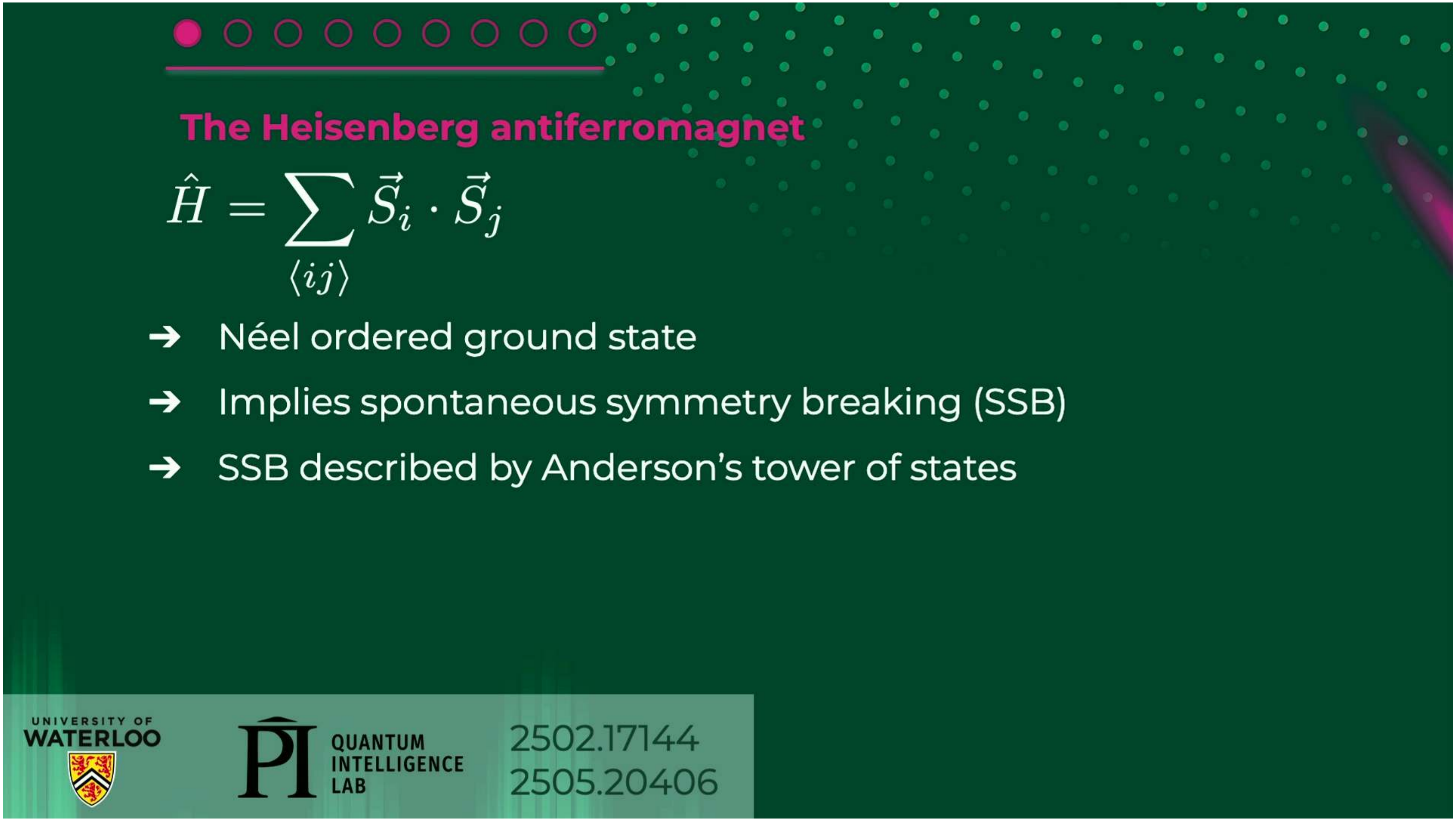
The Heisenberg antiferromagnet
$$\hat{H} = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$
➔ Néel ordered ground state
➔ Implies spontaneous symmetry breaking (SSB)
➔ SSB described by Anderson's tower of states
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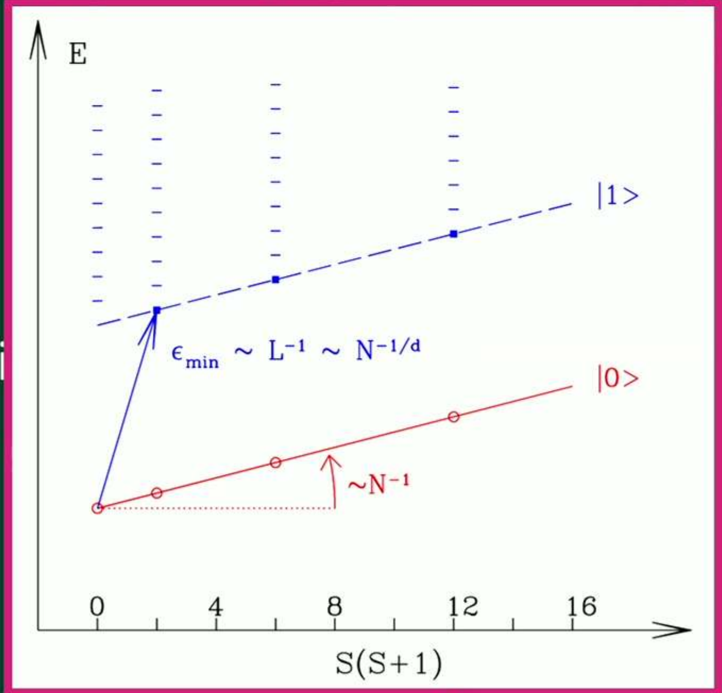

C. Lhuillier, Frustrated Quantum Magnets (2005), arXiv:cond-mat/0502464.

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The Heisenberg antiferromagnet

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- ➔ Néel ordered ground state
- ➔ Implies spontaneous symmetry breaking (SSB)
- ➔ SSB described by Anderson's tower of states
- □ Hamiltonian can be made "stoquastic" with a local unitary
- △ No know local unitary to make Hamiltonian "stoquastic"
- ⧖ Enough frustration to destroy order

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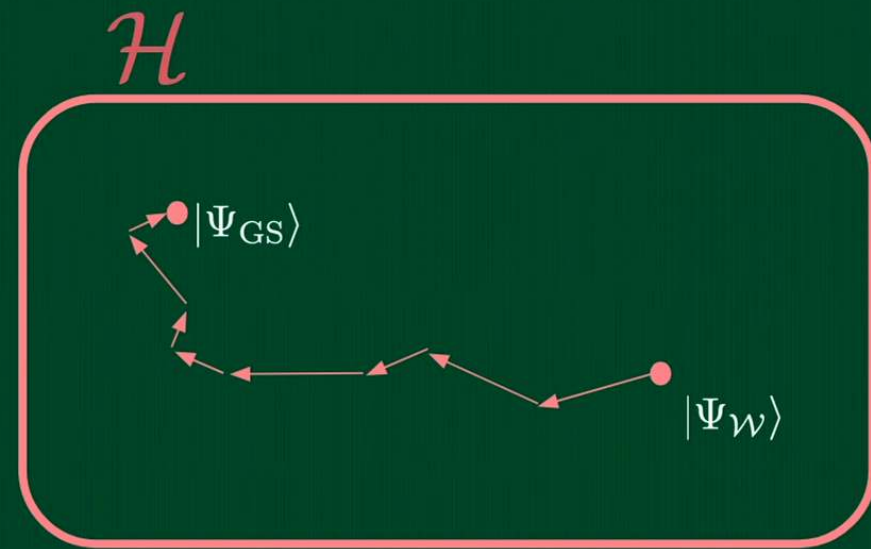
Neural network wavefunctions (Neural quantum states)

$$|\Psi_{\mathrm{GS}}\rangle \in \mathbb{C}^{2^N}$$

$$|\Psi_{\mathcal{W}}\rangle \qquad ||\mathcal{W}|| \ll 2^N$$

$$E_{\mathcal{W}} \equiv \frac{\langle \Psi_{\mathcal{W}} | \hat{H} | \Psi_{\mathcal{W}} \rangle}{\langle \Psi_{\mathcal{W}} | \Psi_{\mathcal{W}} \rangle}$$

$$|\Psi_{\mathcal{W}}\rangle \rightarrow |\Psi_{\mathrm{GS}}\rangle$$



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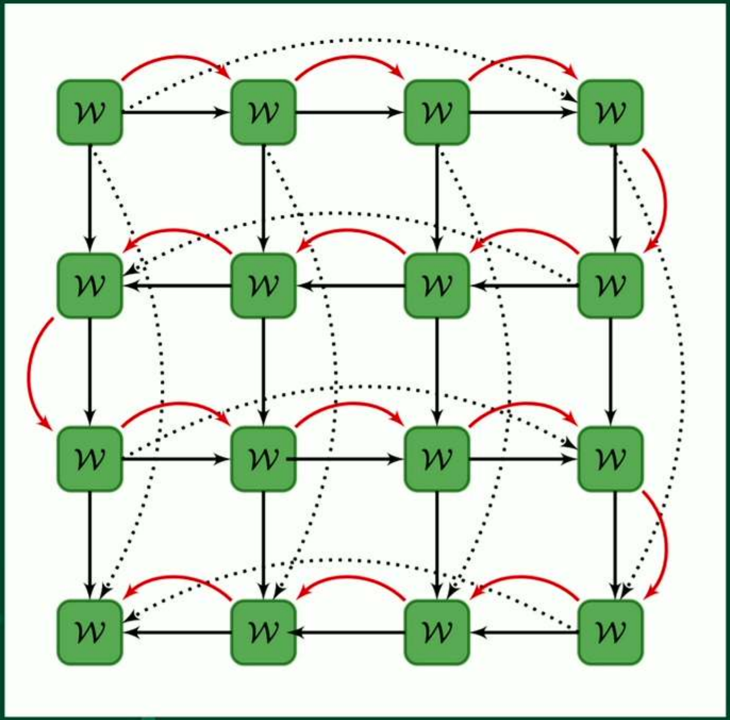
“Leveraging recurrence”



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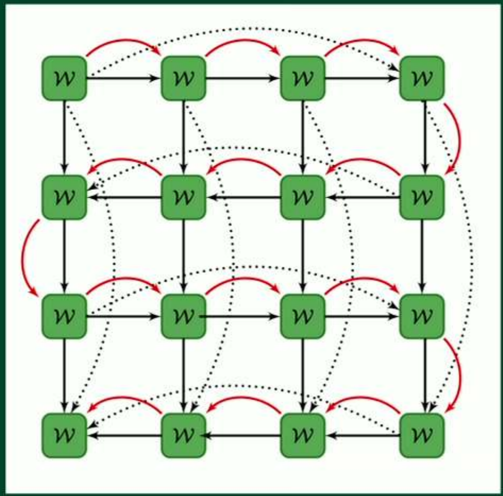
"Leveraging recurrence"

$$\vec{h}_t = f_{\mathcal{W}}(\vec{h}_{t-1}) \quad t = 1 \ldots N$$



- ➔ # parameters is independent of # spins
- ➔ Permits "iterative retraining" (transfer learning across system size)

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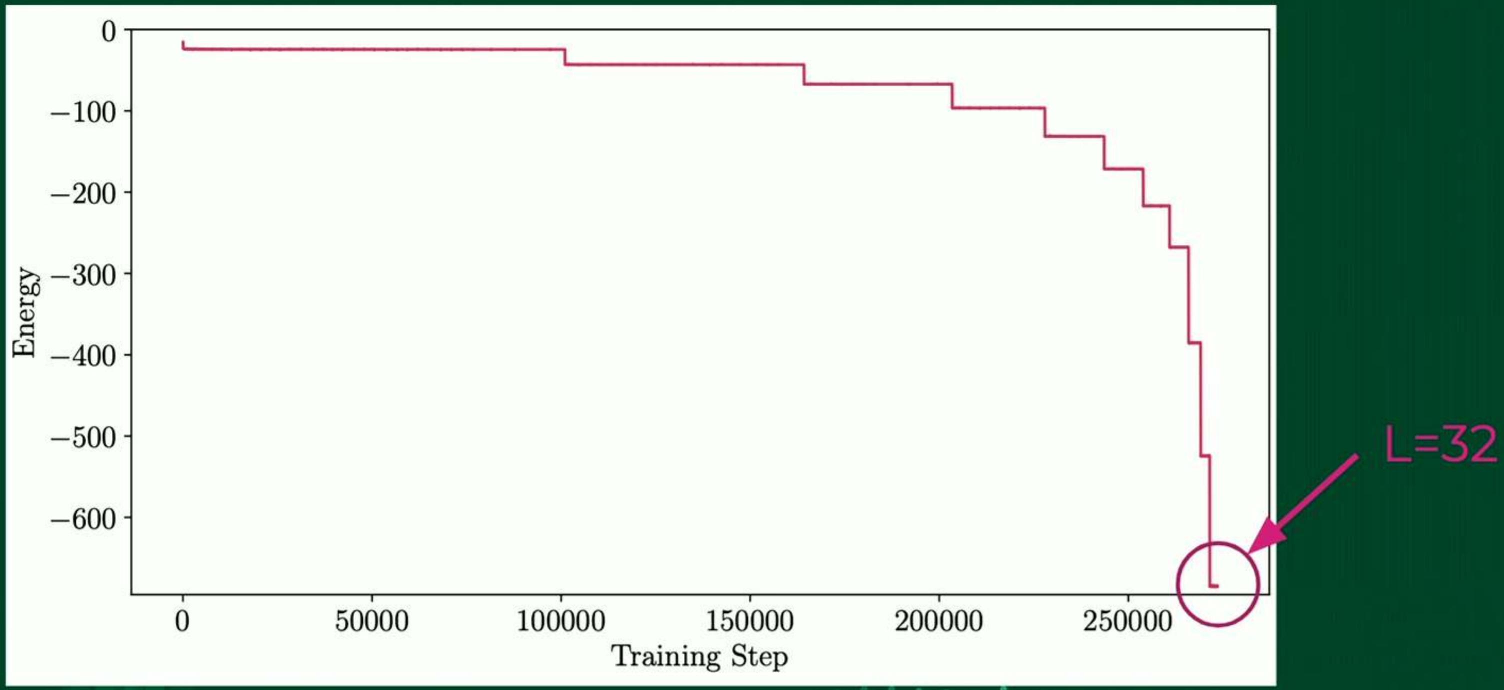
Iterative Retraining



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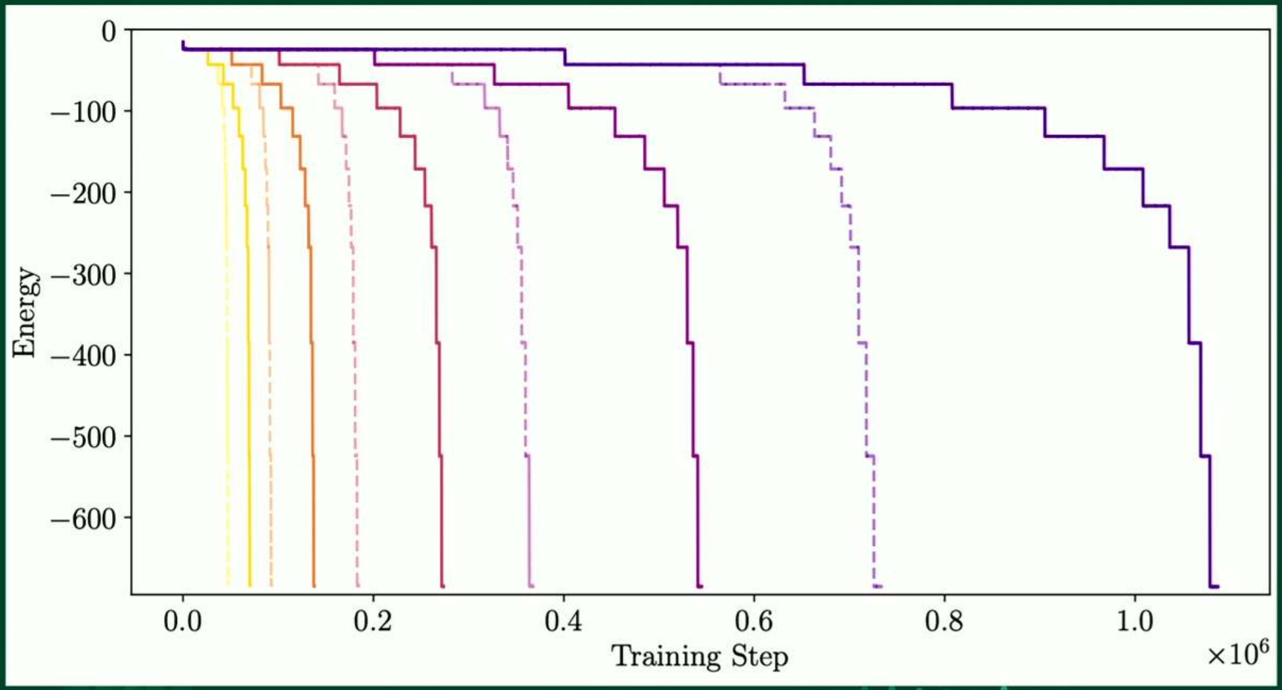
Iterative Retraining



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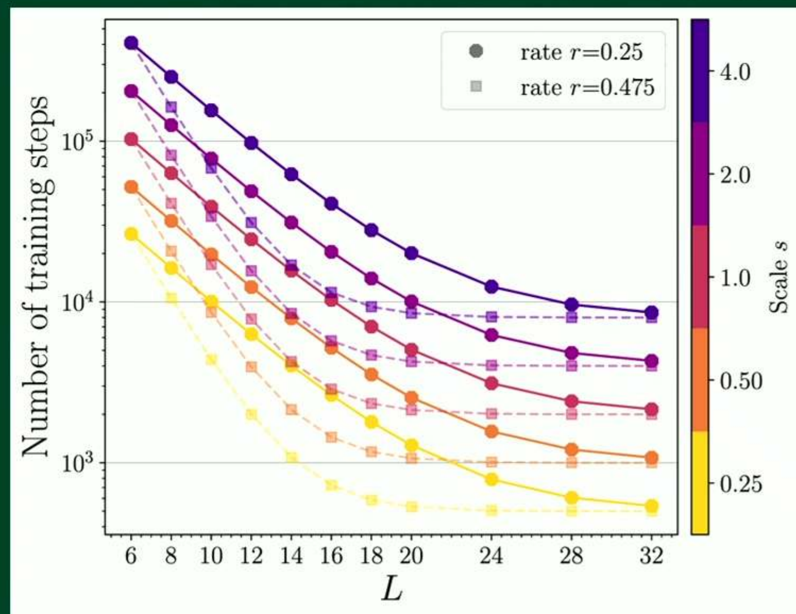
Iterative Retraining



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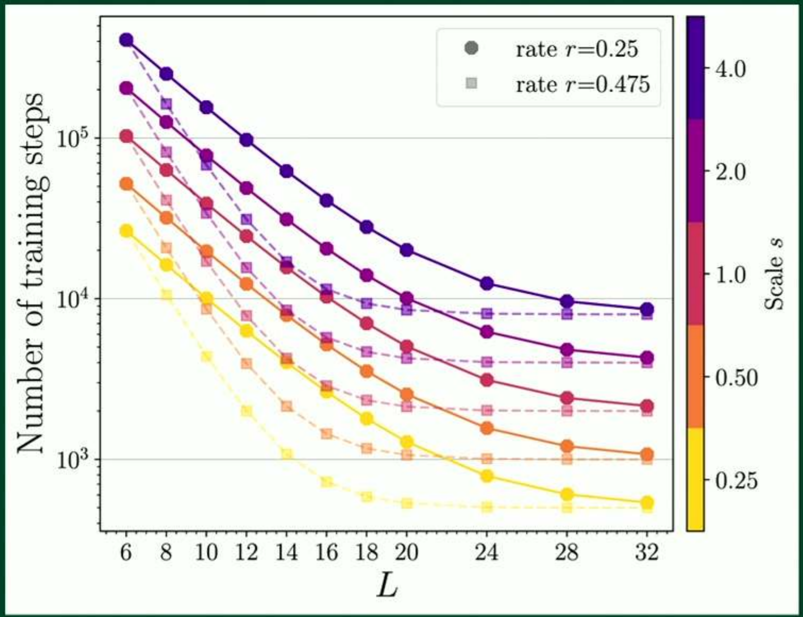
Iterative Retraining



$$N_{\text{steps}}(L, s, r; L_0, C) = s \times [C\exp(-r(L - L_0)) + F]$$

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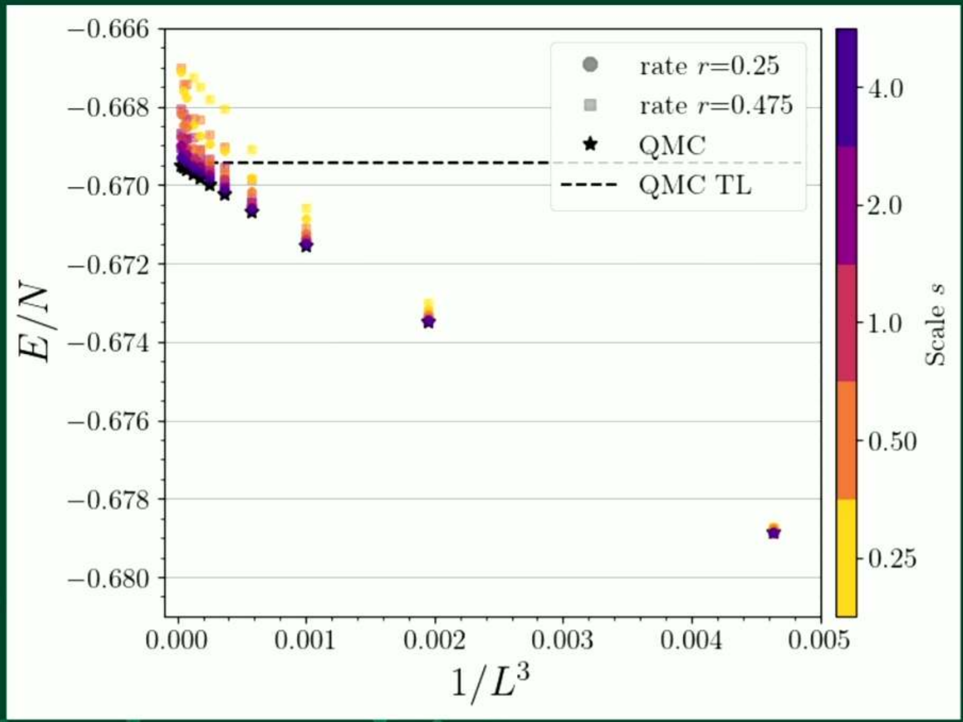
☐ Results: variational energies



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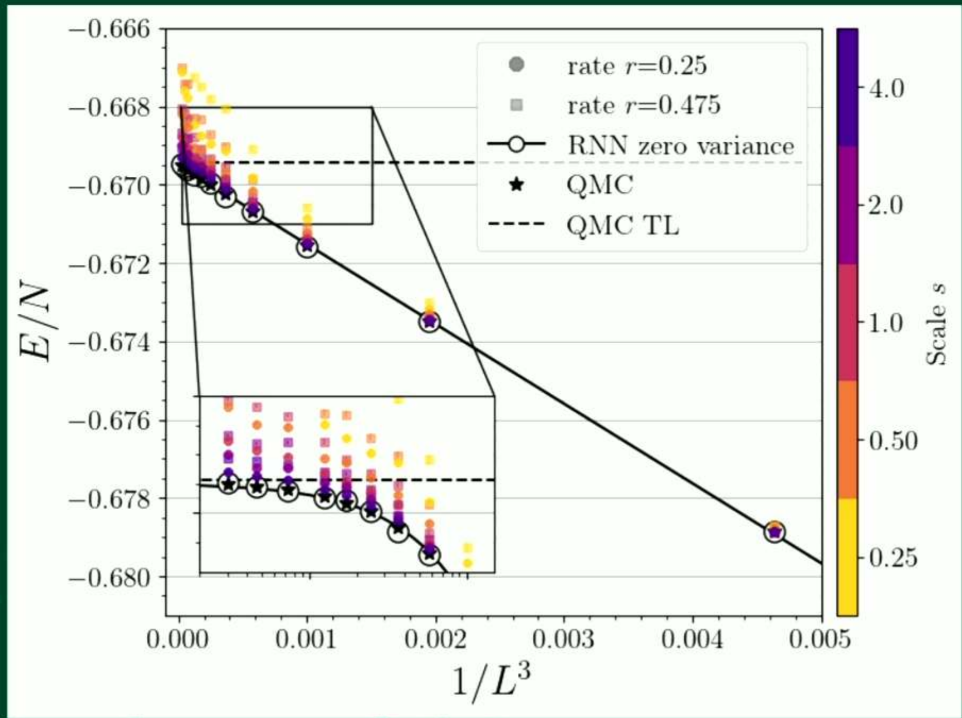
Results: variational energies



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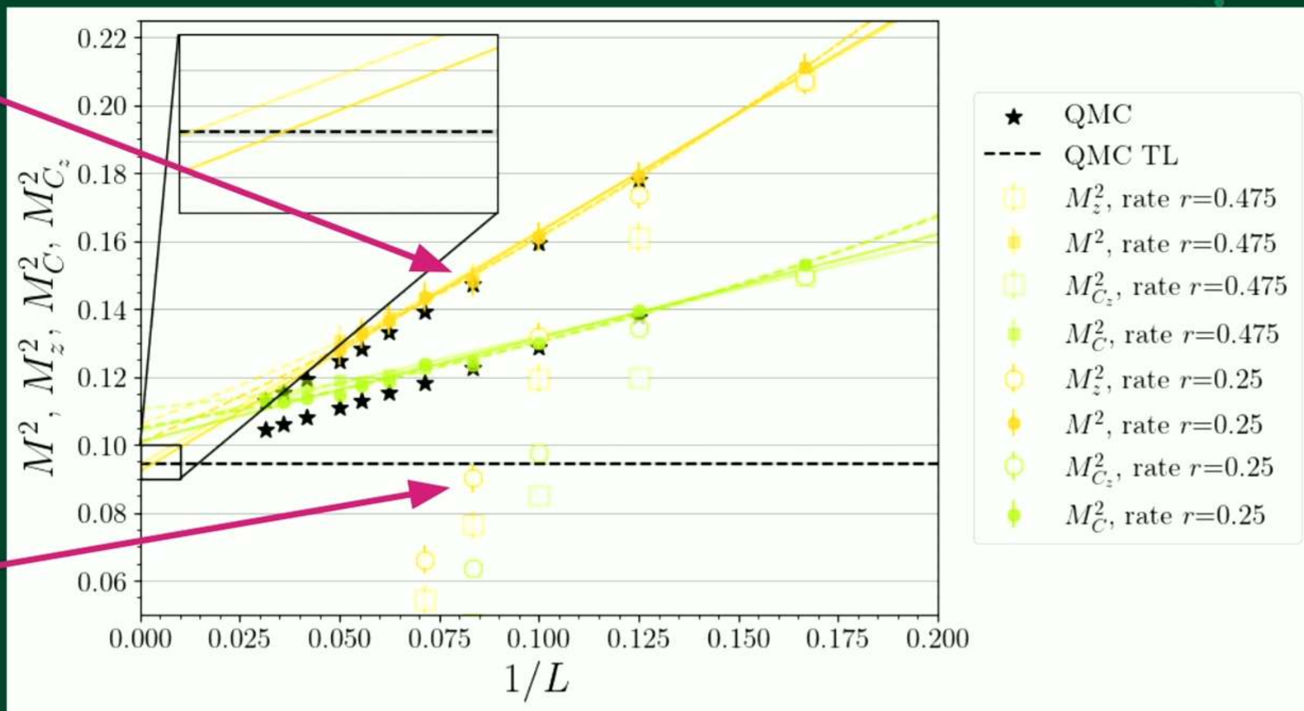
□ Results: sublattice magnetization

$\langle \vec{S}_i \cdot \vec{S}_j \rangle$



$\langle S_i^z S_j^z \rangle$

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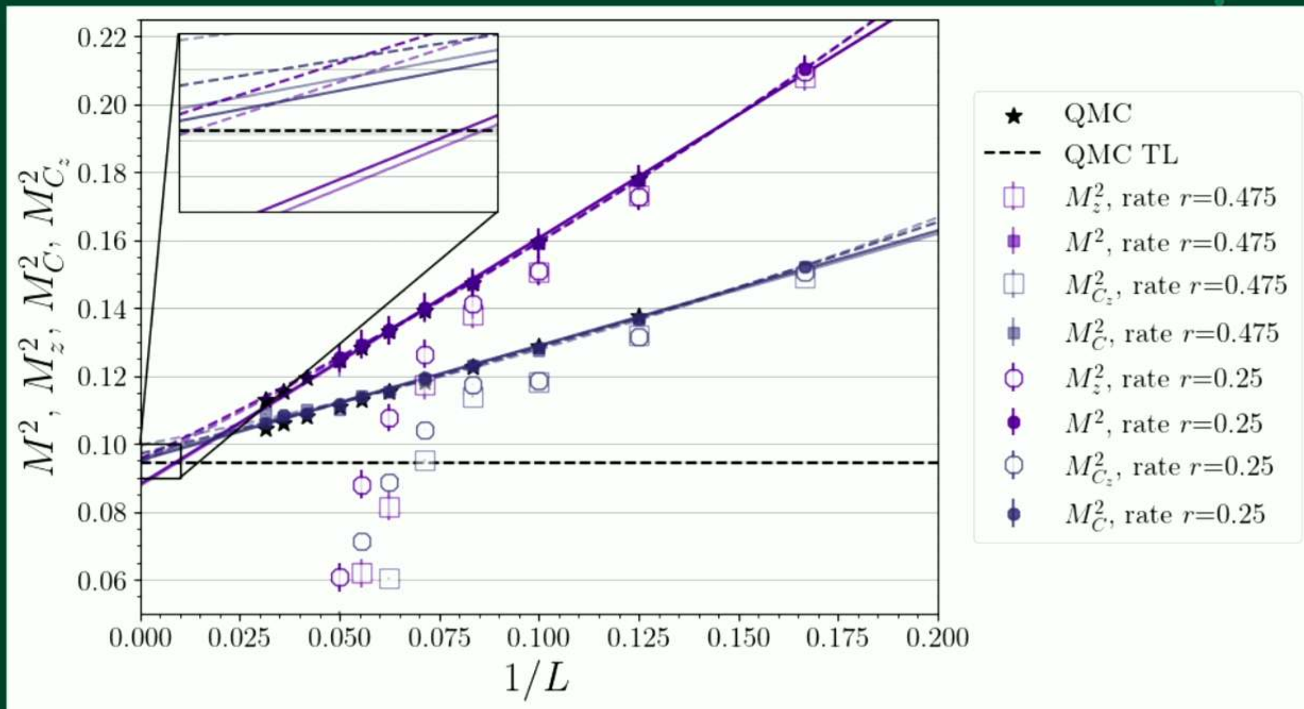
☐ Results: sublattice magnetization



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△ Results: variational energies

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Conclusion & Outlook

- ➔ RNN wavefunctions + iterative retraining are powerful methods for simulating very large systems (allows us to extrapolate to the thermodynamic limit)
- ➔ Knowledge of Anderson's tower of states theoretically supports the accuracy of our results
- ➔ Simulations for the triangular lattice were much more challenging than the square lattice

⌛ What happens for a disordered ground state?

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