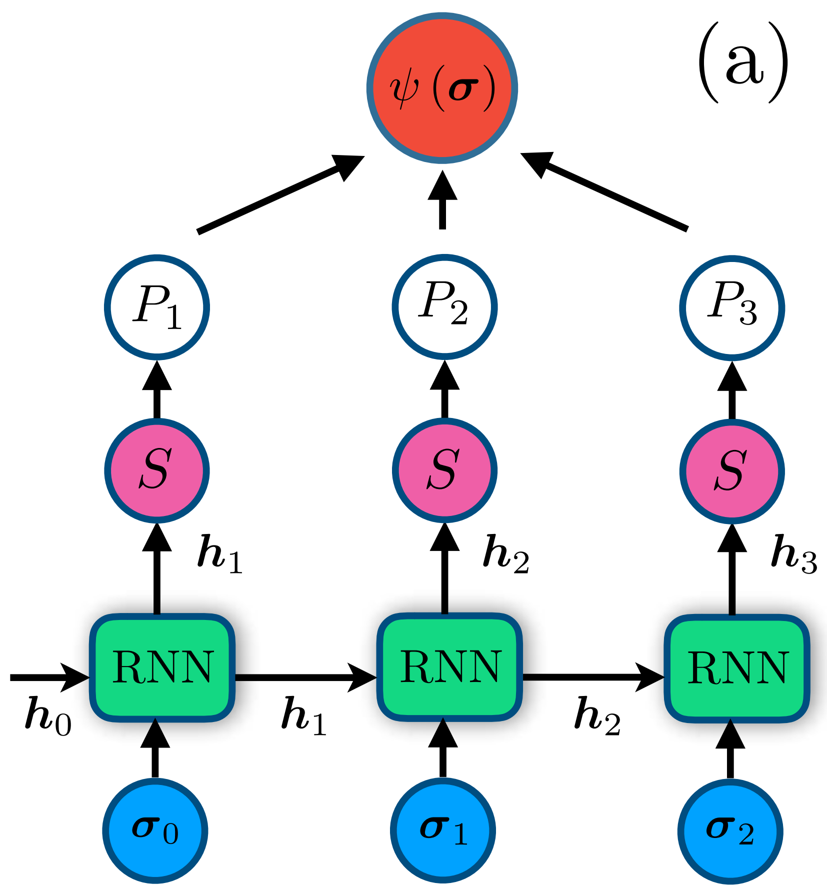
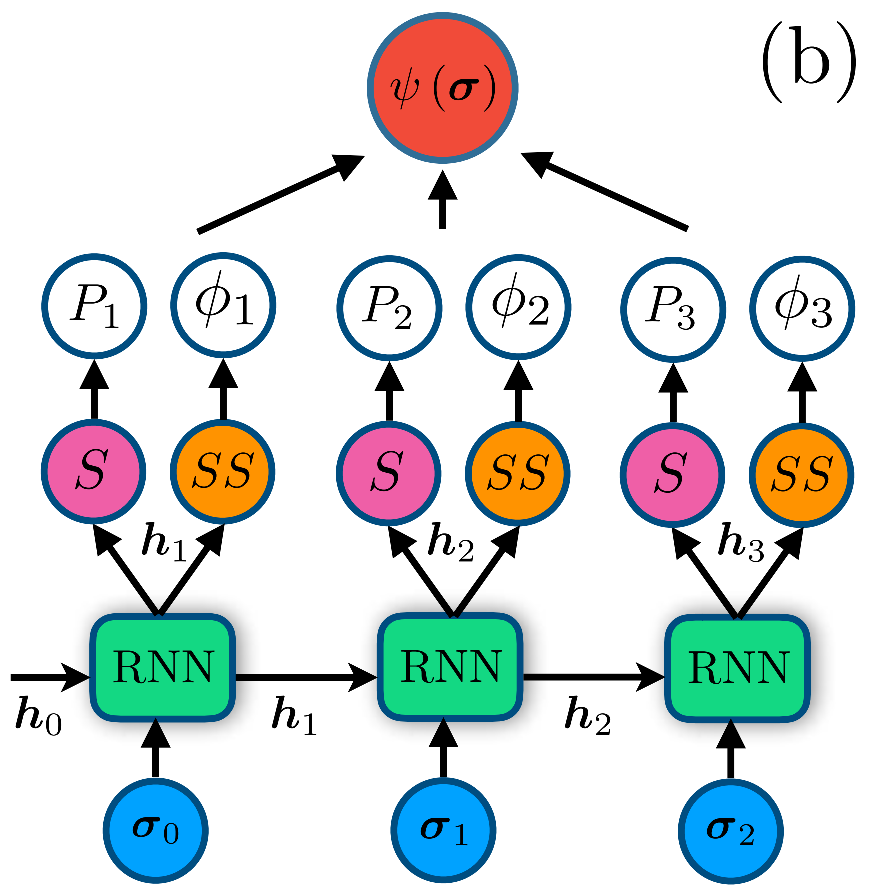
RECURRENT NEURAL NETWORK WAVEFUNCTIONS

2023 Perimeter-SAIFR Journeys into Theoretical Physics

Juan Felipe Carrasquilla Álvarez, July 21st, 2023
Vector Institute

Recurrent neural network wavefunctions

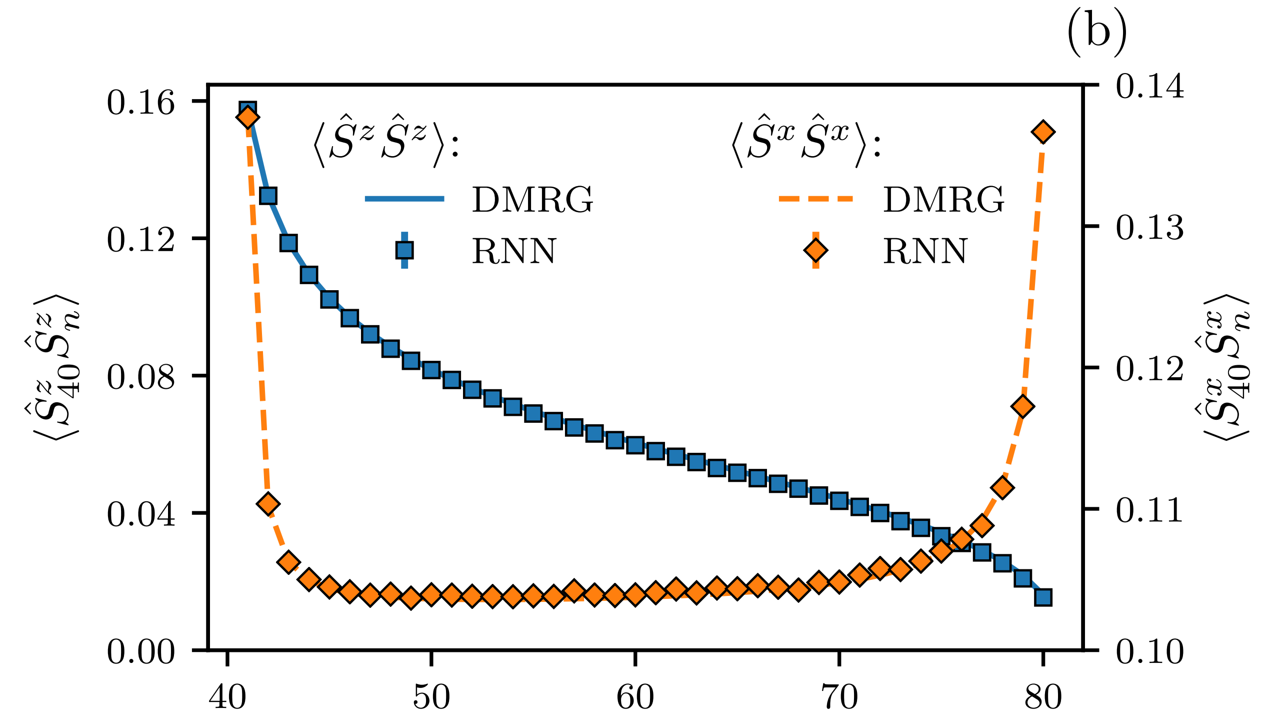




$$|\Psi\rangle = \sum_{\boldsymbol{\sigma}} \psi(\boldsymbol{\sigma})\,|\boldsymbol{\sigma}\rangle = \sum_{\boldsymbol{\sigma}} \sqrt{P(\boldsymbol{\sigma})}\,|\boldsymbol{\sigma}\rangle$$

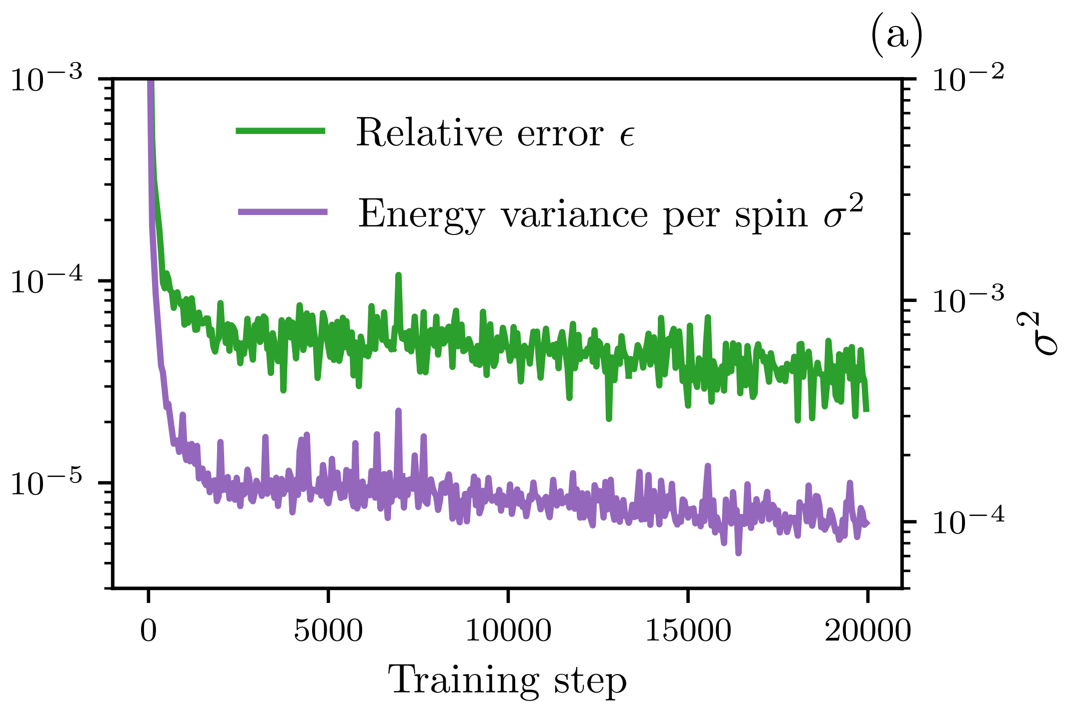
$$|\Psi\rangle = \sum_{\boldsymbol{\sigma}} \exp(\mathrm{i}\phi(\boldsymbol{\sigma}))\sqrt{P(\boldsymbol{\sigma})}\,|\boldsymbol{\sigma}\rangle$$

$$\mathcal{H} = J\sum_{ij}\sigma_i^z\sigma_j^z + h\sum_i \sigma_i^x$$



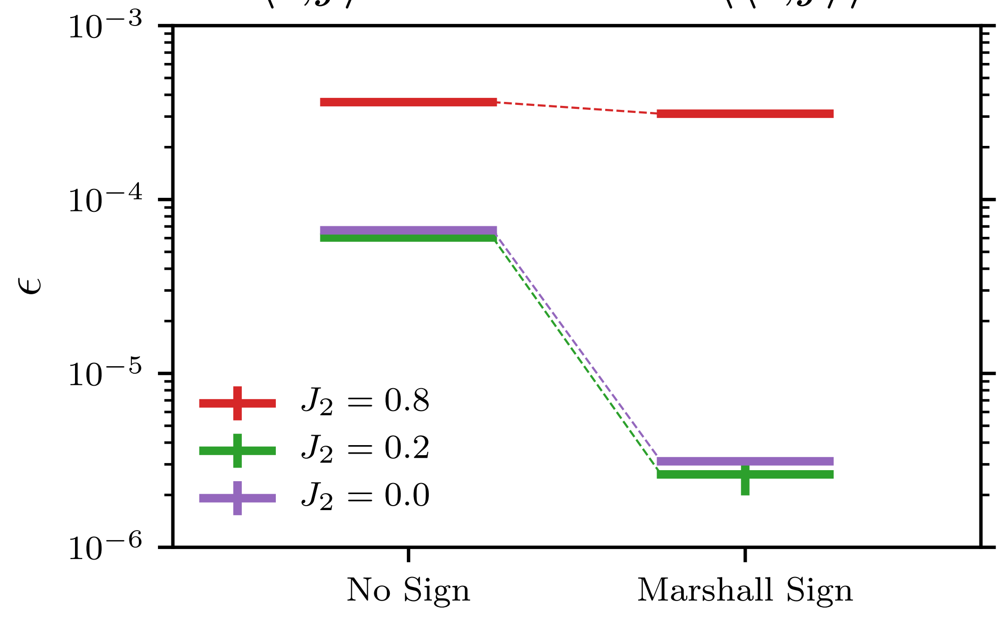
TFIM 1-D N=80

$$\mathcal{H} = J\sum_{ij}\sigma_i^z\sigma_j^z + h\sum_i \sigma_i^x$$

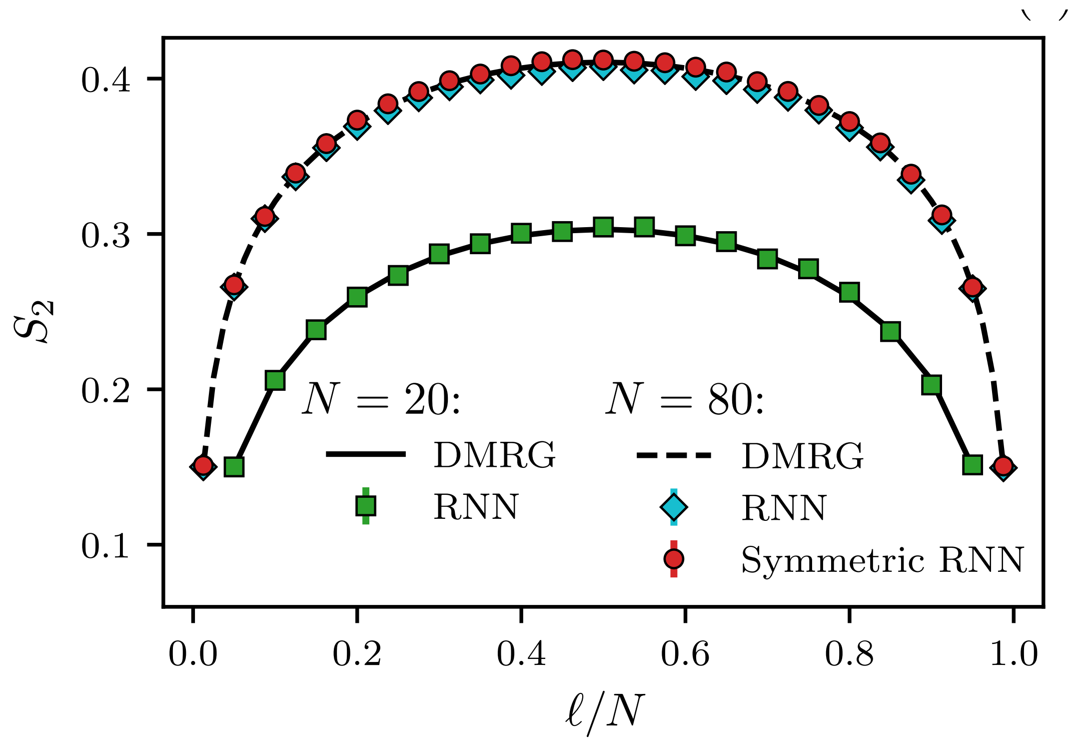


TFIM 1-D N=1000

$$H = J_1\sum_{\langle i,j\rangle} S_i.S_j + J_2\sum_{\langle\langle i,j\rangle\rangle} S_i.S_j$$



J1-J2 model in 1-D

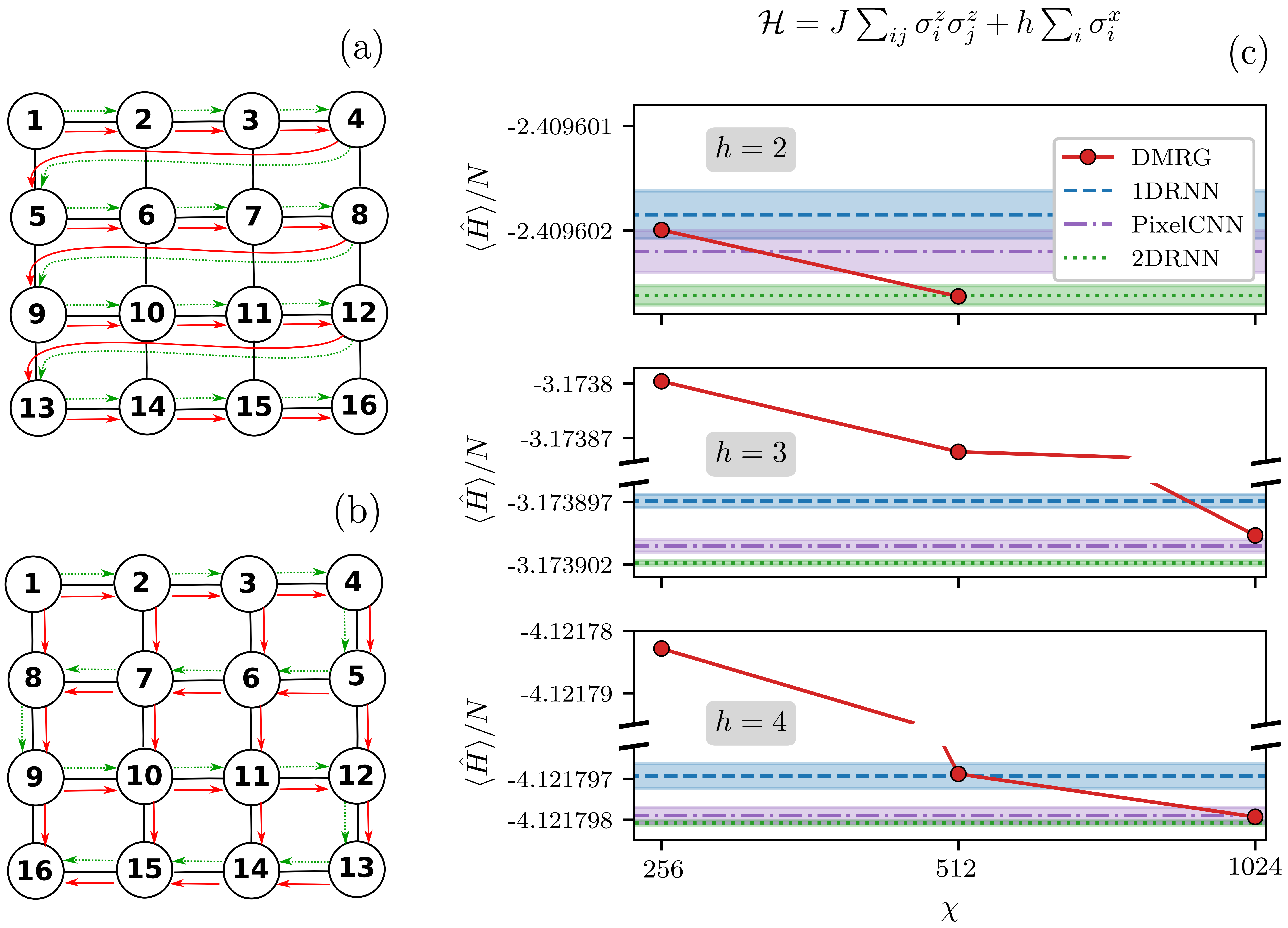


TFIM 1-D N=80

Symmetries: Spin inversion, mirror reflection, Sz. Sign: different Marshall signs for the J1-J2 model

Mohamed Hibat-Allah, Martin Ganahl, Lauren E. Hayward, Roger G. Melko, and Juan Carrasquilla Phys. Rev. Research **2**, 023358 (2020)

RECURRENT NEURAL NETWORK WAVEFUNCTIONS IN 2 DIMENSIONS



Mohamed Hibat-Allah, Martin Ganahl, Lauren E. Hayward, Roger G. Melko, and Juan Carrasquilla. Phys. Rev. Research **2**, 023358 (2020)

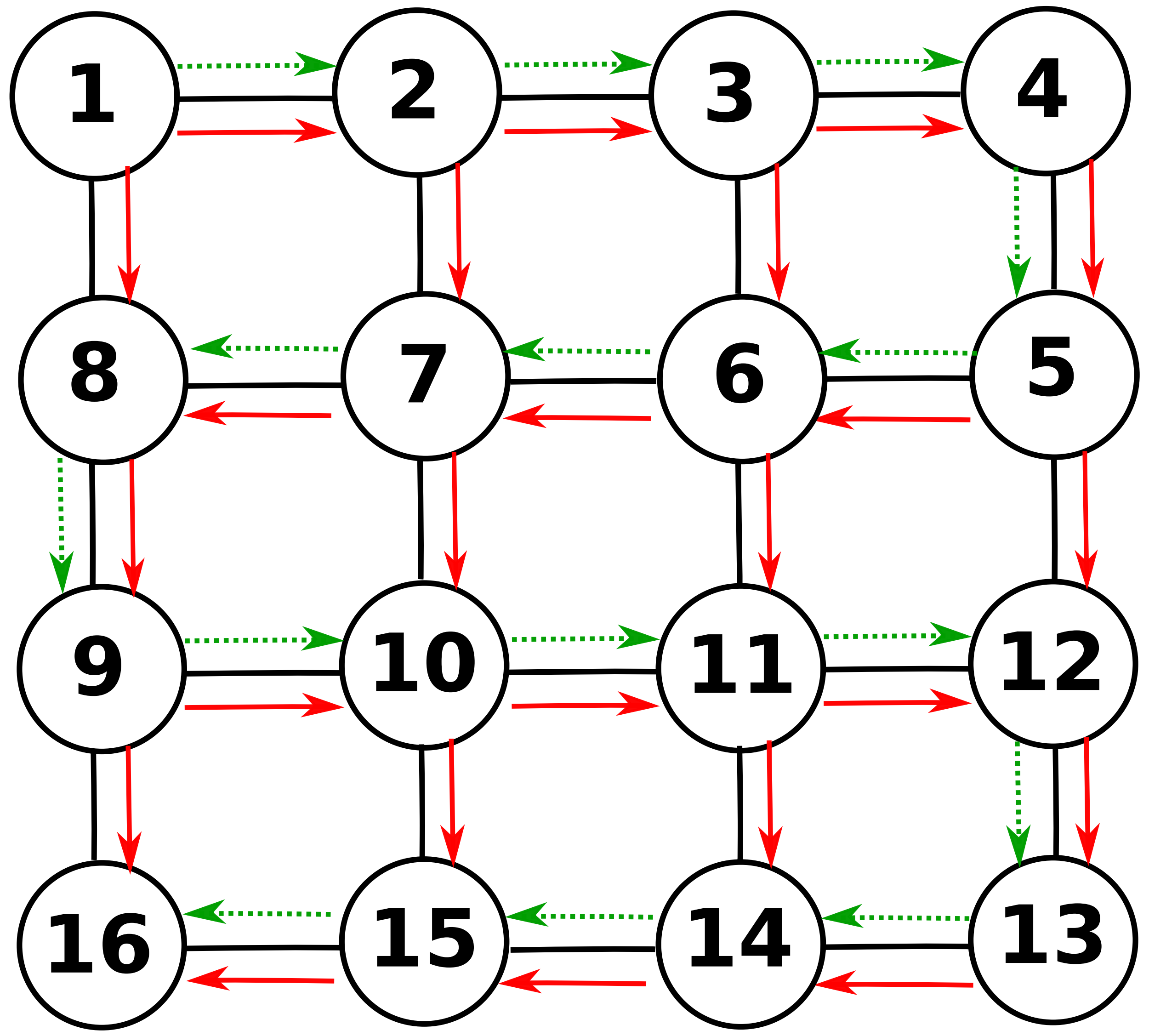
Heinseberg model on the square lattice

$$H = J \sum_{\langle i,j \rangle} S_i . S_j$$

10x10 open boundaries

QMC (Phys. Rev. B 90, 064425): -251.46248

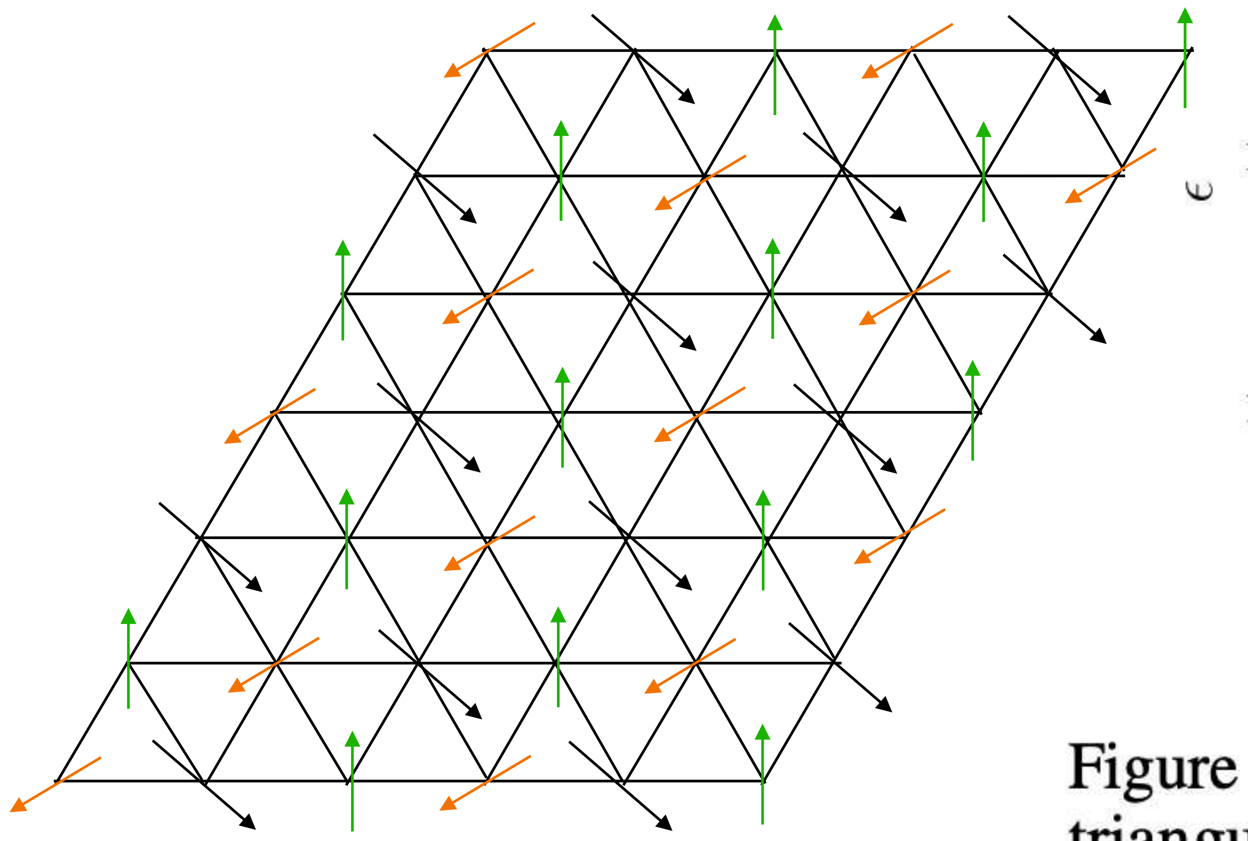
2D RNN: -251.45538 +\- 0.00044

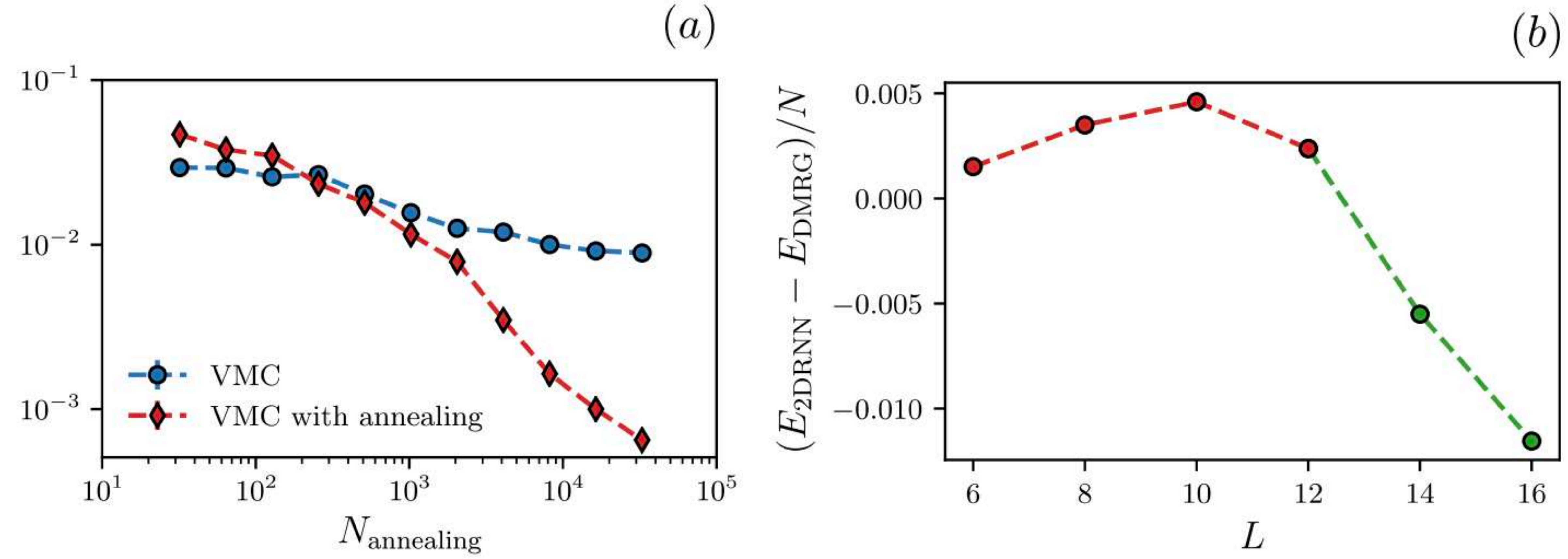


$$\boldsymbol{h}_{i,j} = f\left(W^{(h)}[\boldsymbol{h}_{i-1,j}; \boldsymbol{\sigma}_{i-1,j}] + W^{(v)}[\boldsymbol{h}_{i,j-1}; \boldsymbol{\sigma}_{i,j-1}] + \boldsymbol{b}\right)$$

Mohamed Hibat-Allah, Roger G. Melko, Juan Carrasquilla. Supplementing Recurrent Neural Network Wave Functions with Symmetry and Annealing to Improve Accuracy. Machine Learning and the Physical Sciences, NeurIPS 2021, arXiv:2207.14314

Heinseberg model on the triangular lattice





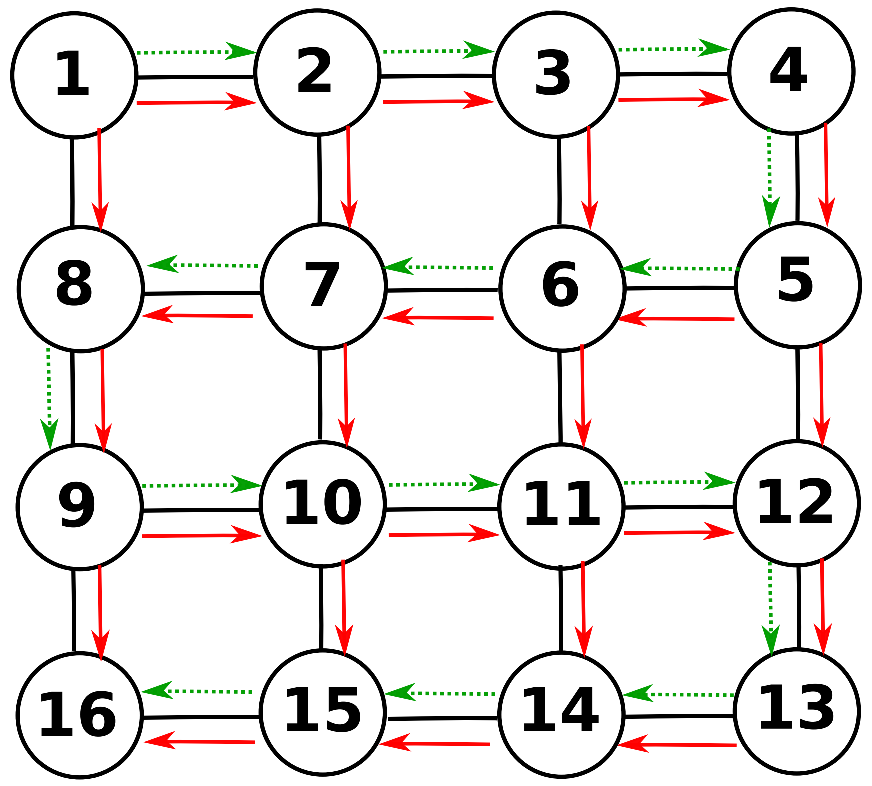
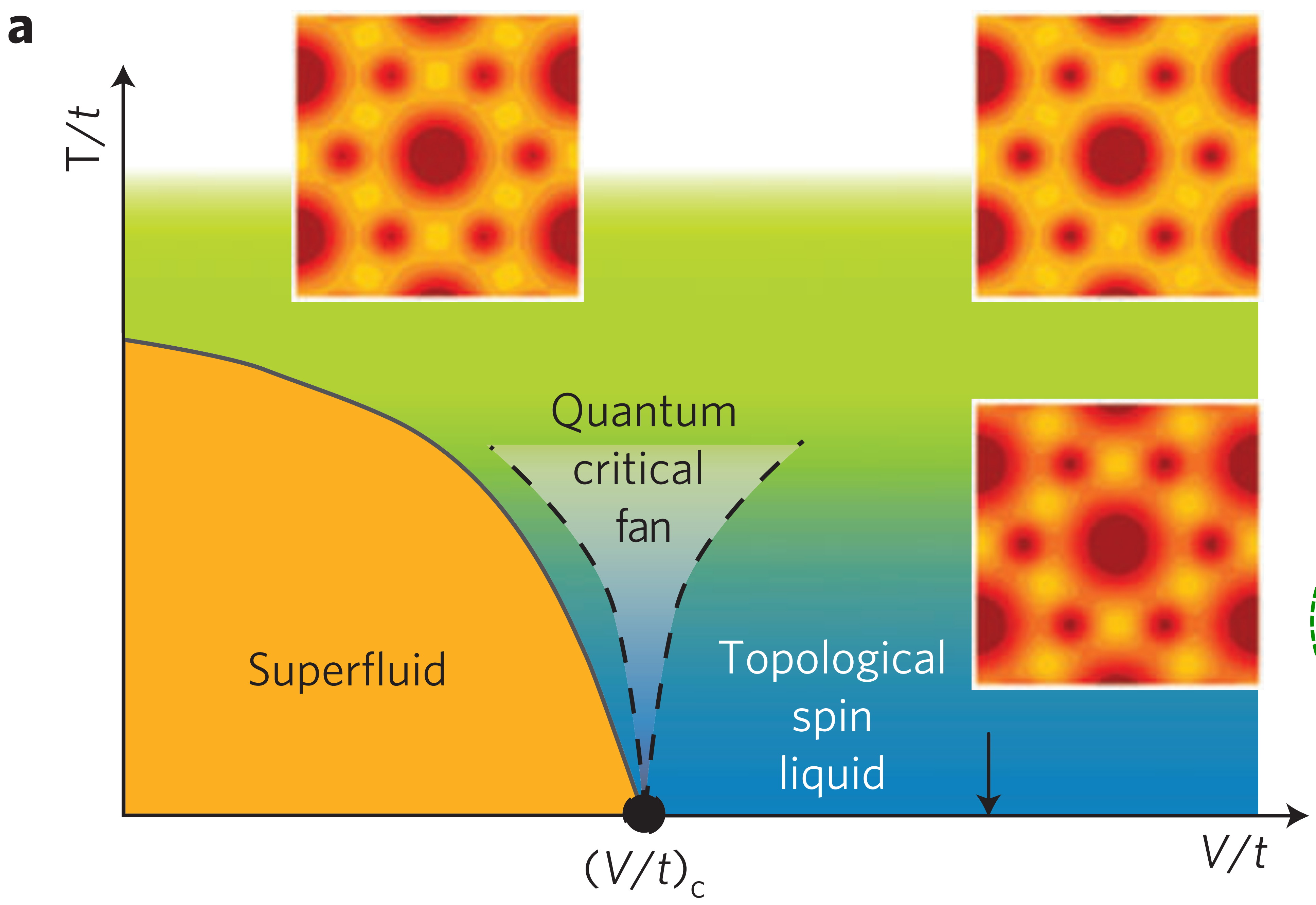


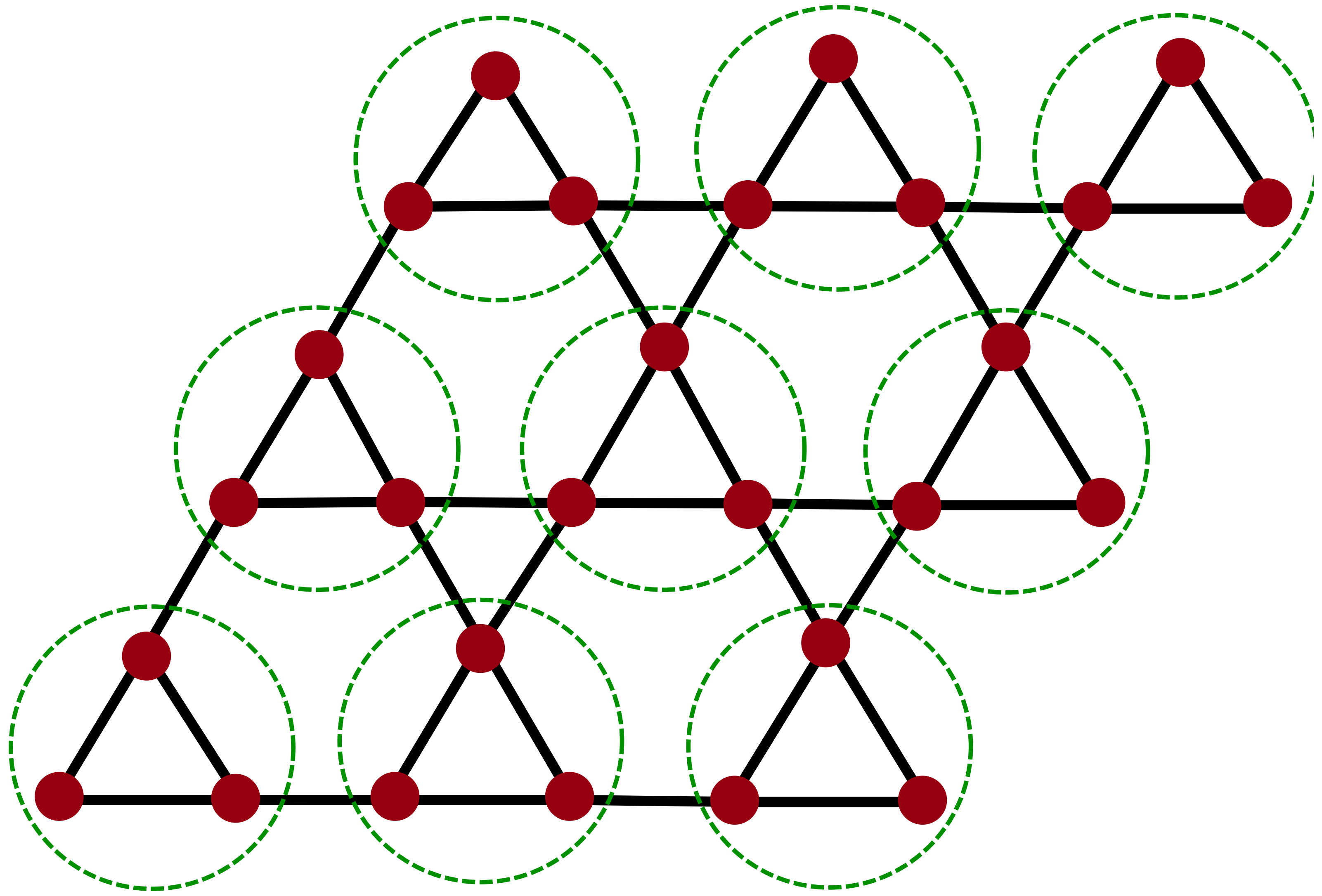
Figure 3: (a) A scaling of the relative error ϵ against the number of annealing steps $N_{\text{annealing}}$ for the triangular Heisenberg model with size 4×4, ‘VMC’ corresponds to an initial pseudo-temperature $T_0 = 0$ whereas for ‘VMC with annealing’, we start with $T_0 = 1$. (b) A plot of the energy difference per site between the 2DRNN and the DMRG. Negative values show that our ansatz is superior compared to DMRG for system sizes larger than 14×14.

RNN wavefunction better than DMRG for large systems. Uses 0.1% of parameters compared to DMRG (D=2K,3K)

Topological entanglement entropy of a Bose–Hubbard spin liquid

$$\hat{H} = -\sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + b_i b_j^\dagger \right) + V \sum_{\hexagon} n_{\hexagon}^2 \qquad n_{\hexagon} = \sum_{i \in \hexagon} (n_i - 1/2)$$

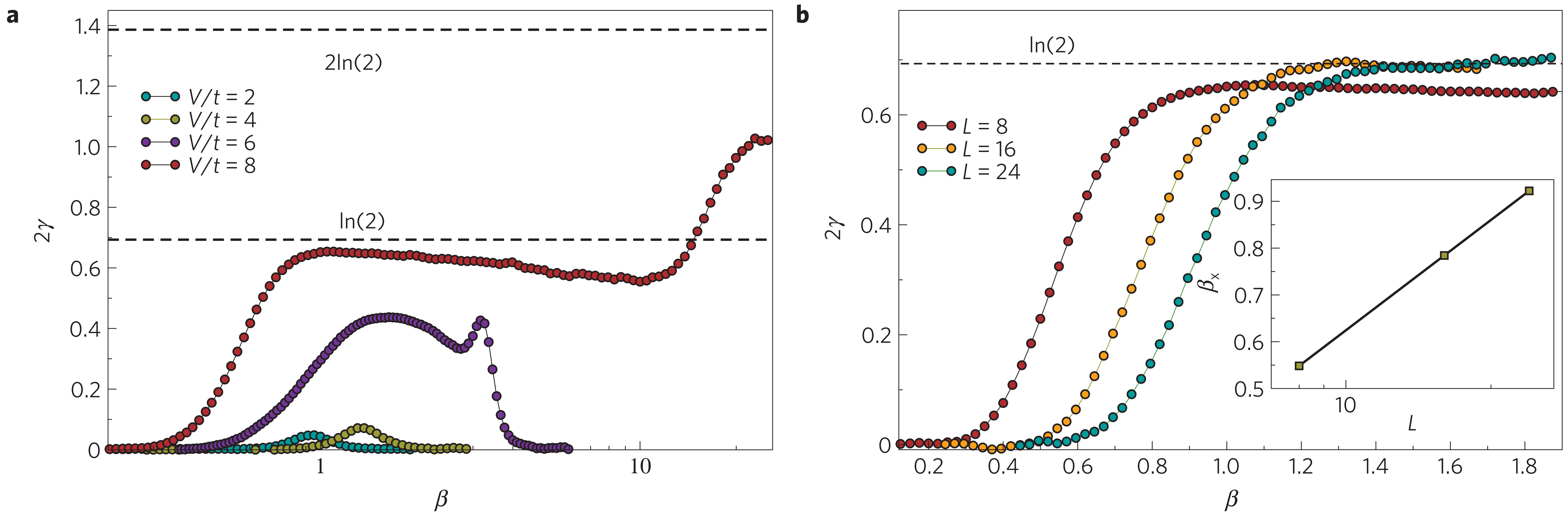




Sergei V. Isakov, Matthew B. Hastings & Roger G. Melko Nature Physics volume 7, pages 772–775 (2011)

Topological entanglement entropy

QMC based on stochastic series expansion



- $\gamma = \log(2)$— QMC can't reach low enough temperatures for this system to saturate γ to the value predicted by field theory.

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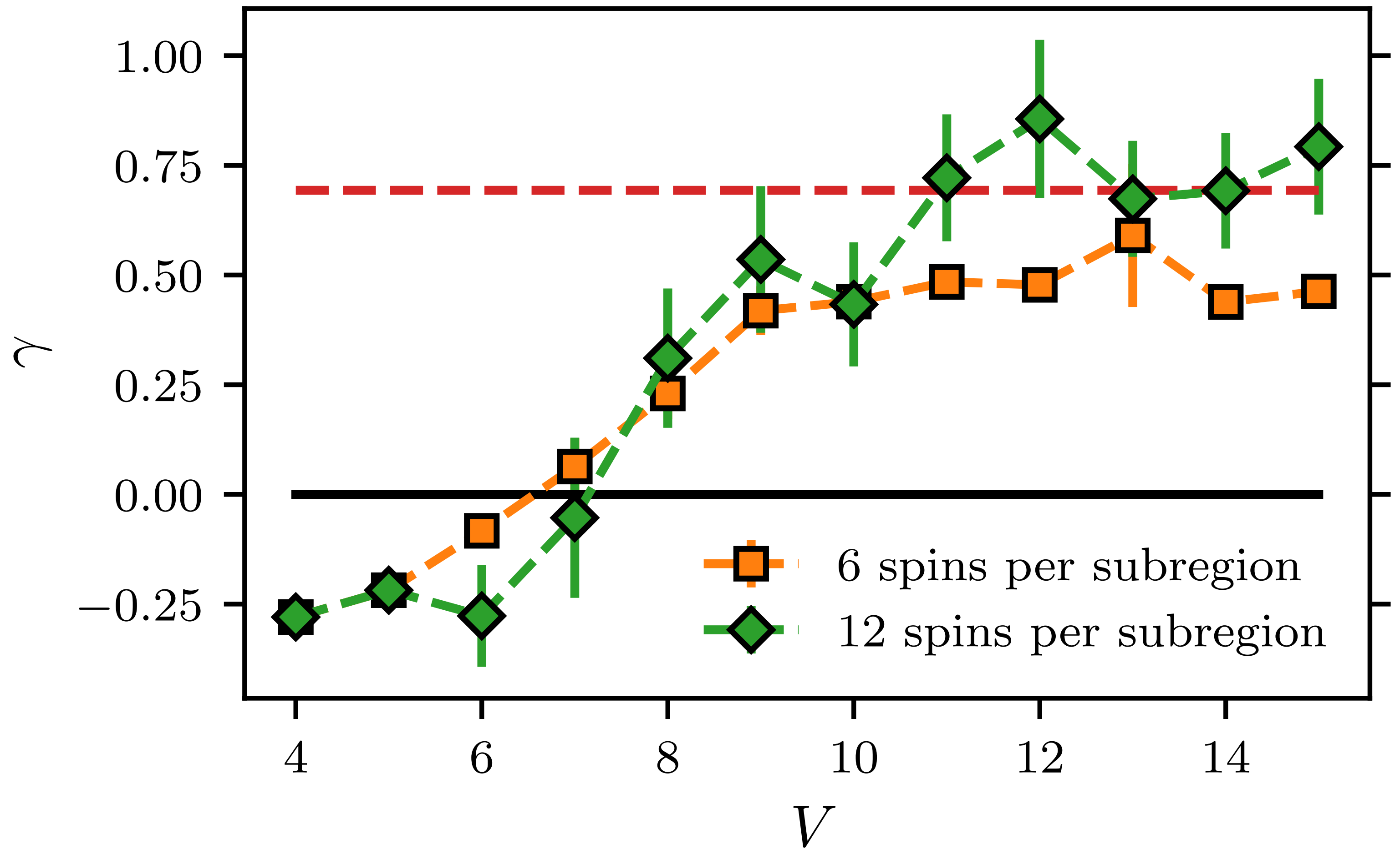
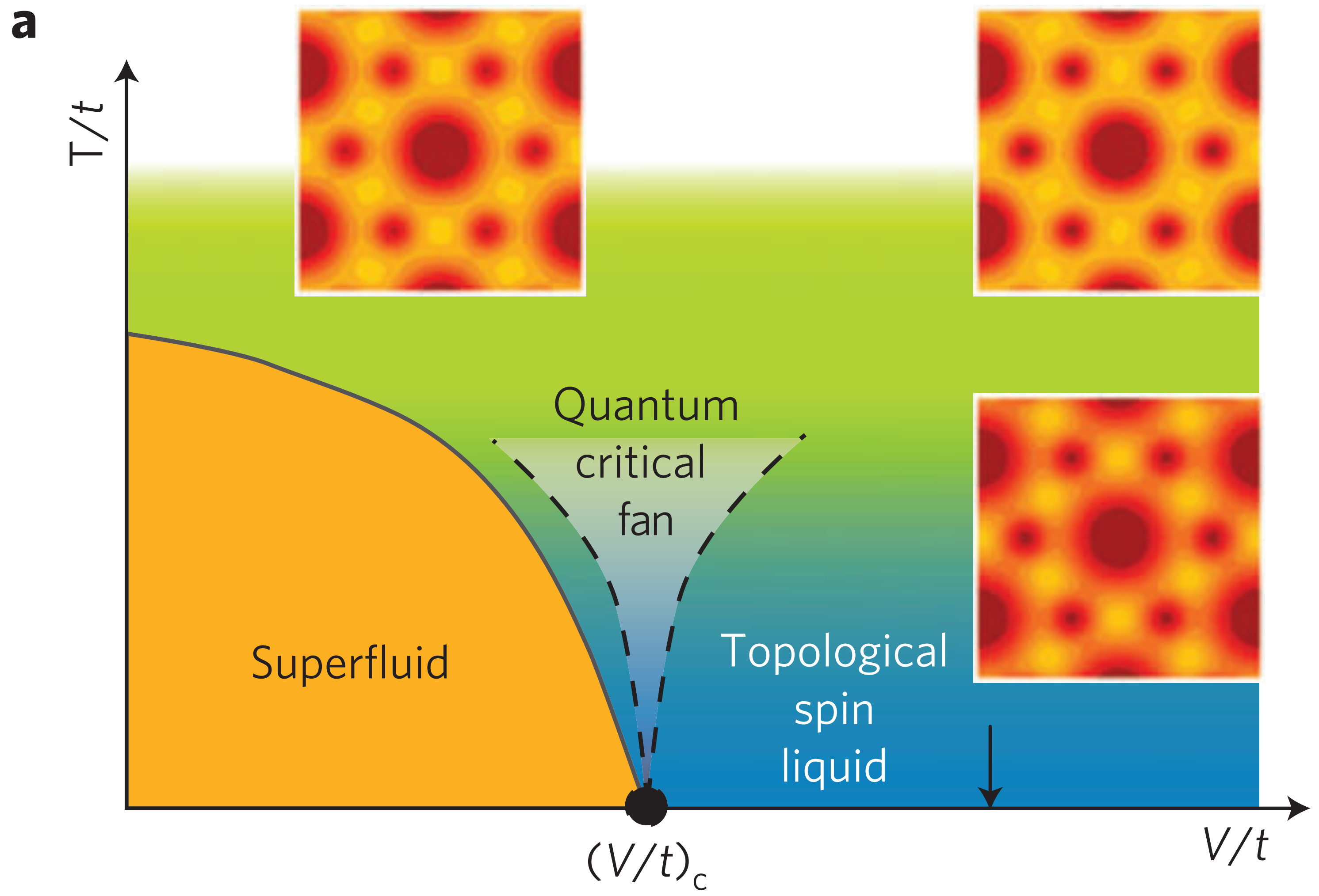
Variational calculation using annealing RNN

- RNN ansatz





Kitaev-Preskill construction—