Title: Investigating Topological Order with Recurrent Neural Network Wave Functions

Speakers: Mohamed Hibat Allah

Collection: Machine Learning for Quantum Many-Body Systems

Date: June 14, 2023 - 2:30 PM

URL: https://pirsa.org/23060039

Abstract: Recurrent neural networks (RNNs), originally developed for natural language processing, hold great promise for accurately describing strongly correlated quantum many-body systems. In this talk, we will illustrate how to use 2D RNNs to investigate two prototypical quantum many-body Hamiltonians exhibiting topological order. Specifically, we will demonstrate that RNN wave functions can effectively capture the topological order of the toric code and a Bose-Hubbard spin liquid on the kagome lattice by estimating their topological entanglement entropies. Overall, we will show that RNN wave functions constitute a powerful tool for studying phases of matter beyond Landau's symmetry-breaking paradigm.

Investigating Topological Order with Recurrent Neural Network Wave Functions

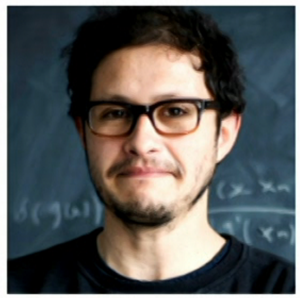
Mohamed Hibat-Allah

Machine Learning for Quantum Many-Body Physics

14th of June 2023

arXiv:2303.11207

Acknowledgments

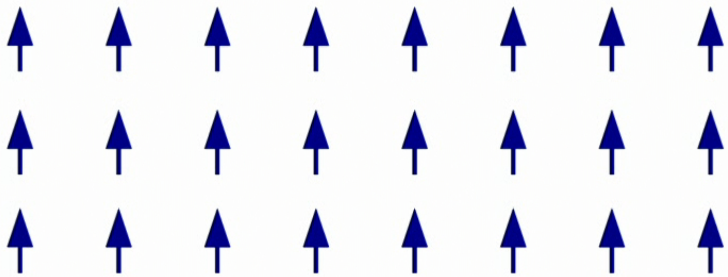


Juan
Carrasquilla

Roger
Melko

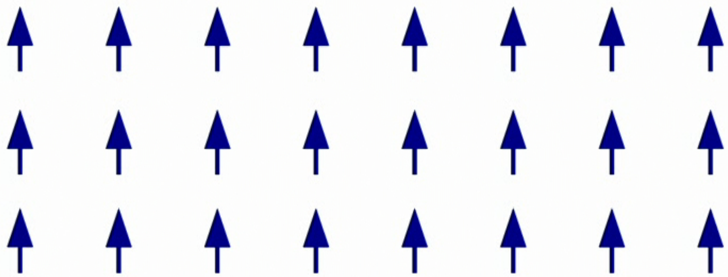
Investigating topological order using RNN wave functions, arXiv:2303.11207, Mar 2023

Phases of matter

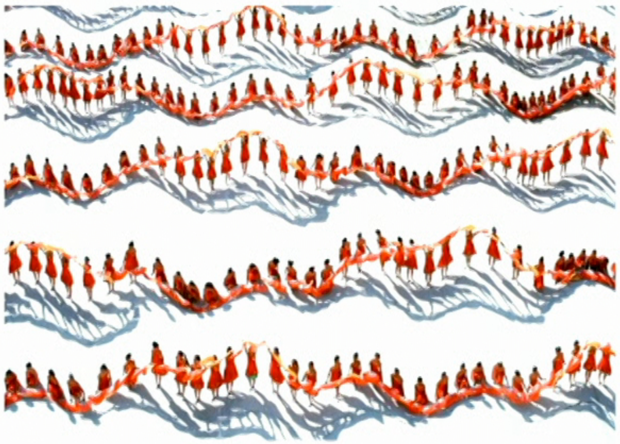


Ferromagnet (non topological – local)
(credit: Michael Schmidt)

Phases of matter



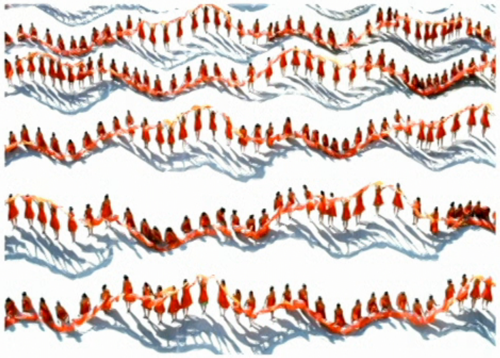
Ferromagnet (non topological – local)
(credit: Michael Schmidt)



Spin liquid (topological – nonlocal)
(credit: Xiao-Gang Wen)

Why studying topological order?

- Zero-temperature phase of quantum matter.
  - Fractional Quantum Hall effect.
  - Fault-tolerant quantum computation.
  - Quantum Spin liquids.



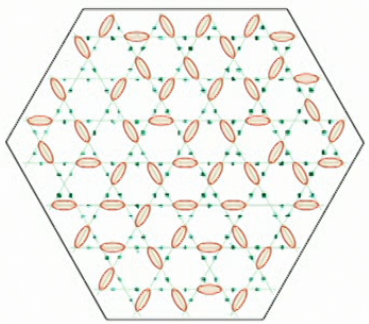
Credit: Xiao-Gang Wen

Experimental realizations of topological order

TOPOLOGICAL MATTER

Probing topological spin liquids on a programmable quantum simulator

G. Semeghini[1], H. Levine[1], A. Keesling[1,2], S. Ebadi[1], T. T. Wang[1], D. Bluvstein[1], R. Verresen[1], H. Pichler[3,4], M. Kalinowski[1], R. Samajdar[1], A. Omran[1,2], S. Sachdev[1,5], A. Vishwanath[1*], M. Greiner[1*], V. Vuletić[6*], M. D. Lukin[1*]

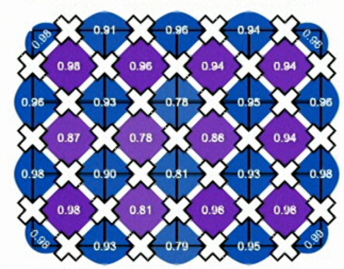


Topological order in Rydberg atom arrays

TOPOLOGICAL MATTER

Realizing topologically ordered states on a quantum processor

K. J. Satzinger[1*], Y.-J Liu[2,3], A. Smith[2,4,5], C. Knapp[6,7†], M. Newman[1], C. Jones[1], Z. Chen[1], C. Quintana[1], X. Mi[1], A. Dunsworth[1], C. Gidney[1], I. Aleiner[1], F. Arute[1], K. Arya[1], J. Atalaya[1], R. Babbush[1], J. C. Bardin[1,8], R. Barends[1], J. Basso[1], A. Bengtsson[1], A. Bilmes[1], M. Broughton[1], B. B. Buckley[1], D. A. Buell[1], B. Burkett[1], N. Bushnell[1], B. Chiaro[1], R. Collins[1], W. Courtney[1], S. Demura[1], A. R. Derk[1], D. Eppens[1], C. Erickson[1], L. Faoro[9], E. Farhi[1], A. G. Fowler[1], B. Foxen[1], M. Giustina[1], A. Greene[1,10], J. A. Gross[1], M. P. Harrigan[1], S. D. Harrington[1], J. Hilton[1], S. Hong[1], T. Huang[1], W. J. Huggins[1], L. B. Ioffe[1], S. V. Isakov[1], E. Jeffrey[1], Z. Jiang[1], D. Kafri[1], K. Kechedzhi[1], T. Khattar[1], S. Kim[1], P. V. Klimov[1], A. N. Korotkov[1,11], F. Kostritsa[1], D. Landhuis[1], P. Laptev[1], A. Locharla[1], E. Lucero[1], O. Martin[1], J. R. McClean[1], M. McEwen[1,12], K. C. Miao[1], M. Mohseni[1], S. Montazeri[1], W. Mruczkiewicz[1], J. Mutus[1], O. Naaman[1], M. Neeley[1], C. Neill[1], M. Y. Niu[1], T. E. O'Brien[1], A. Opremcak[1], B. Pató[1], A. Petukhov[1], N. C. Rubin[1], D. Sank[1], V. Shvarts[1], D. Strain[1], M. Szalay[1], B. Villalonga[1], T. C. White[1], Z. Yao[1], P. Yeh[1], J. Yoo[1], A. Zalcman[1], H. Neven[1], S. Boixo[1], A. Megrant[1], Y. Chen[1], J. Kelly[1], V. Smelyanskiy[1], A. Kitaev[1,6,7], M. Knap[2,3,13], F. Pollmann[2,3*], P. Roushan[1*]



Topological order in a superconducting quantum processor

Question?

How machine learning can be used to assist the current efforts of realizing and investigating topological quantum matter?

Question?

Can we detect topological order using neural quantum states?

Question?

Can we detect topological order using recurrent neural network wave functions?

Outline

- 1 - Recurrent Neural Network wave functions.
- 2 - Topological order detection.
- 3 - Promising results on prototypical quantum models.

1 - Recurrent Neural Network

wave functions

Curse of dimensionality in language

The complexity of generating a paragraph of 30 words (assume a dictionary size of 1000 words):

$$1000^{30} \approx 10^{90} \gg \text{number of atoms in our known universe}$$

Curse of dimensionality in language modeling is as challenging compared to (quantum) many-body systems.

Yet, language models can still perform very well!

GPT-4 Technical Report

OpenAI*

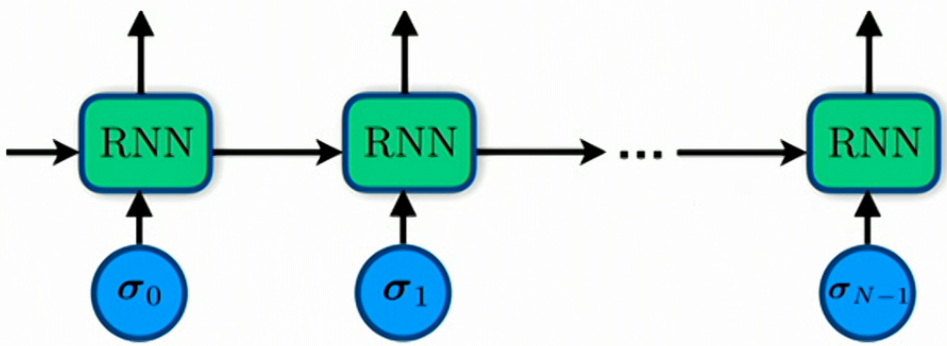
Abstract

We report the development of GPT-4, a large-scale, multimodal model which can accept image and text inputs and produce text outputs. While less capable than humans in many real-world scenarios, GPT-4 exhibits human-level performance on various professional and academic benchmarks, including passing a simulated bar exam with a score around the top 10% of test takers. GPT-4 is a Transformer-based model pre-trained to predict the next token in a document. The post-training alignment process results in improved performance on measures of factuality and adherence to desired behavior. A core component of this project was developing infrastructure and optimization methods that behave predictably across a wide range of scales. This allowed us to accurately predict some aspects of GPT-4's performance based on models trained with no more than 1/1,000th the compute of GPT-4.

GPT-4

ChatGPT

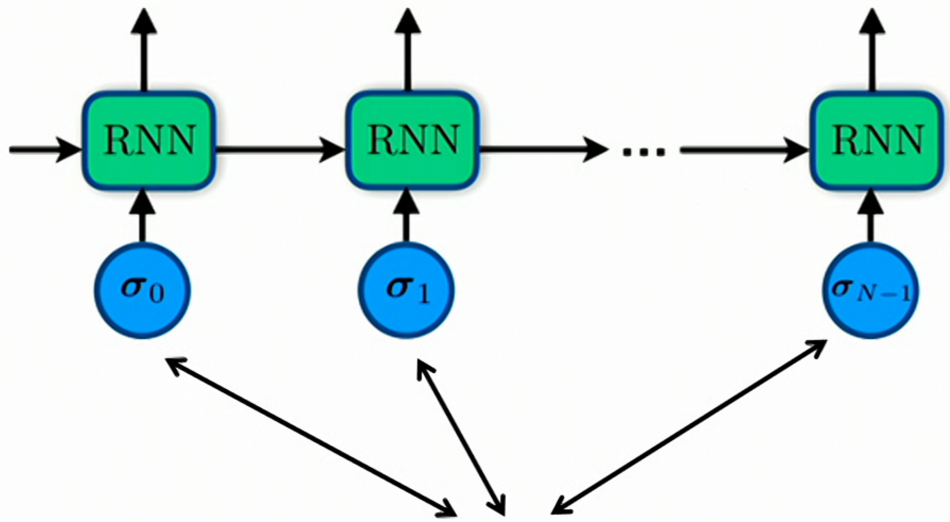
Recurrent Neural Networks (RNNs)



Very powerful at generating sequential data:

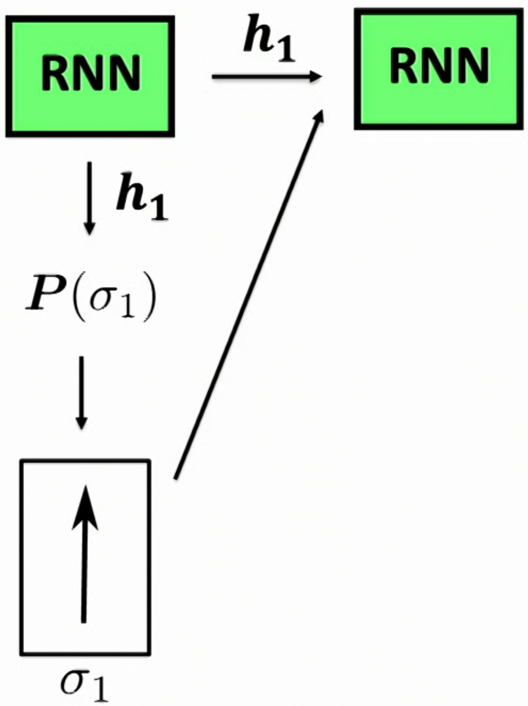
- Speech recognition, machine translation,…

RNNs can be also used in many-body Physics

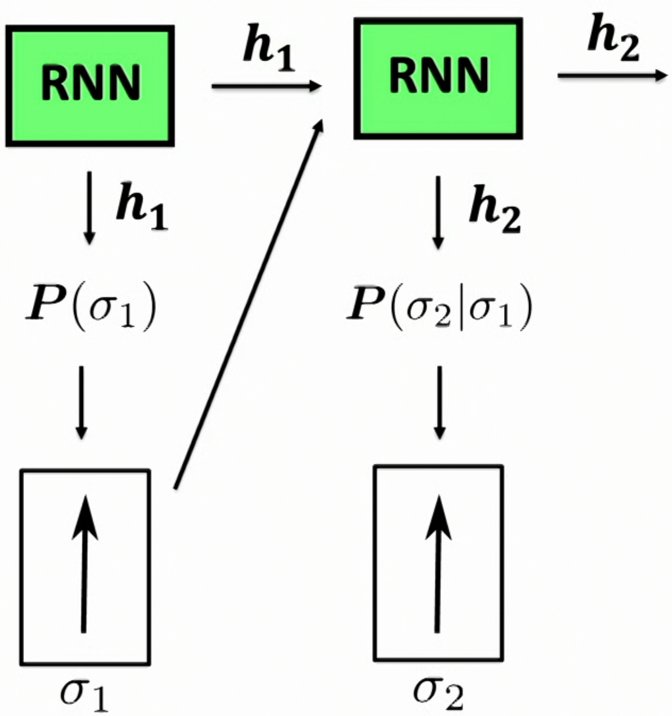


"Spins" instead of "Words"

Autoregressive sampling



Autoregressive sampling



(Simplest) Recursion relation:

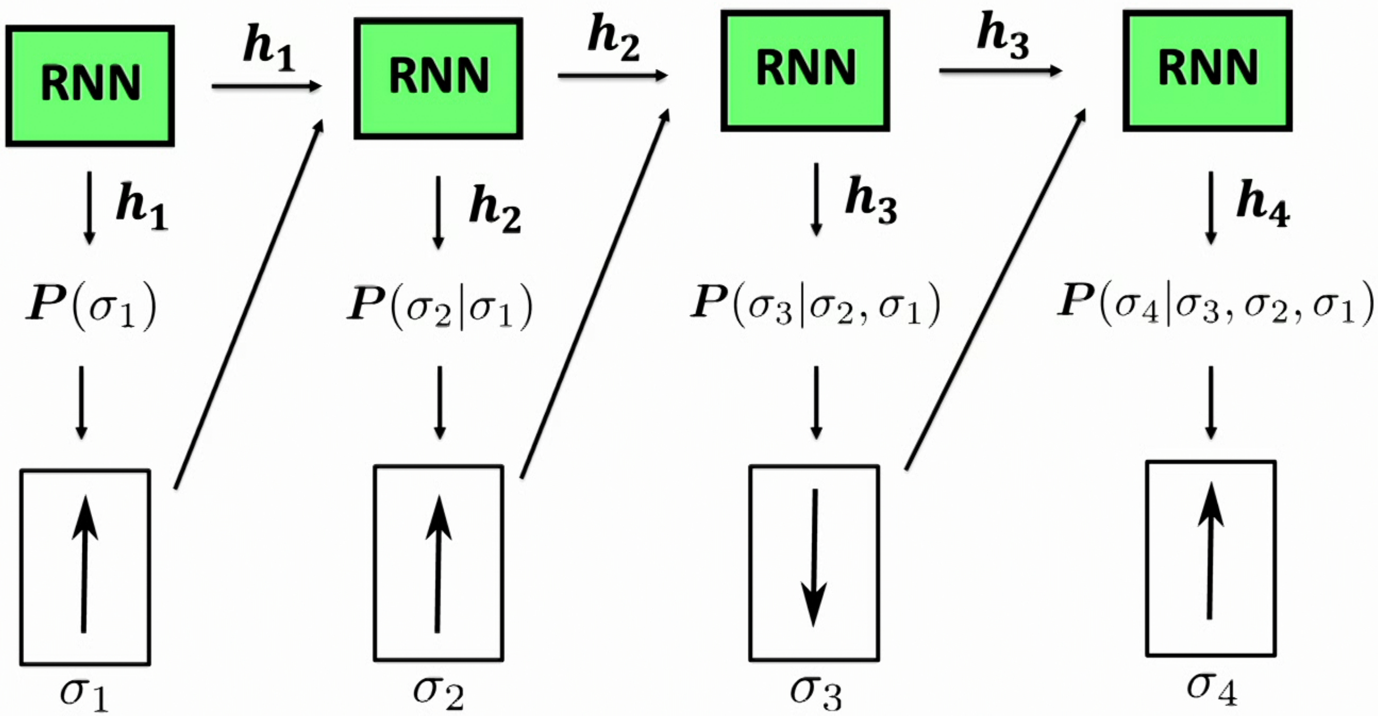
$$\boldsymbol{h}_n = f(W[\boldsymbol{h}_{n-1}; \boldsymbol{\sigma}_{n-1}] + \boldsymbol{b})$$

Conditional probability:

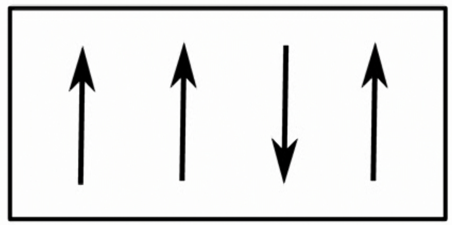
$$\boldsymbol{P}(\sigma_i|\sigma_{<i}) = \textbf{Softmax}(U\boldsymbol{h}_n + \boldsymbol{c}) \cdot \boldsymbol{\sigma}_n$$

***W*, *U*, *b* and *c* are the parameters of the RNN.**

Autoregressive sampling

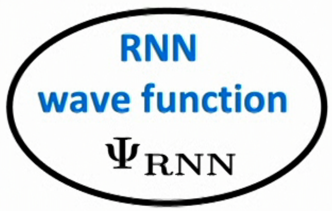


Autoregressive sampling

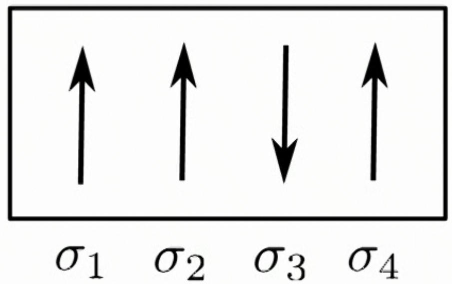


$\sigma_1 \quad \sigma_2 \quad \sigma_3 \quad \sigma_4$

$$|\Psi_{\mathbf{RNN}}(\sigma_1, \sigma_2, \sigma_3, \sigma_4)|^2 = \boldsymbol{P}(\sigma_1)\boldsymbol{P}(\sigma_2|\sigma_1)\boldsymbol{P}(\sigma_3|\sigma_2, \sigma_1)\boldsymbol{P}(\sigma_4|\sigma_3, \sigma_2, \sigma_1)$$



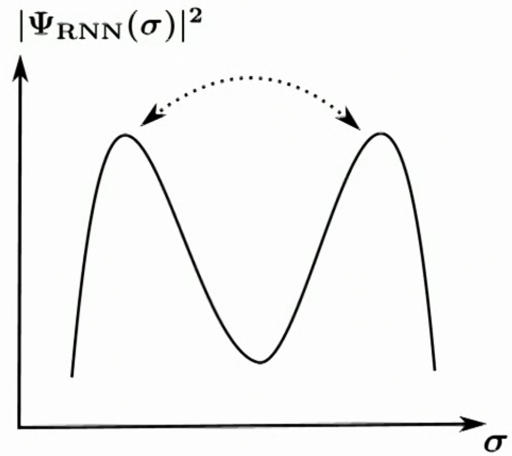
Autoregressive sampling



$$|\Psi_{\mathbf{RNN}}(\sigma_1, \sigma_2, \sigma_3, \sigma_4)|^2 = \boldsymbol{P}(\sigma_1)\boldsymbol{P}(\sigma_2|\sigma_1)\boldsymbol{P}(\sigma_3|\sigma_2, \sigma_1)\boldsymbol{P}(\sigma_4|\sigma_3, \sigma_2, \sigma_1)$$

The samples are independents and can be generated in parallel $\{\boldsymbol{\sigma}^{(j)}\}_{i=1}^{N_s}$

Autoregressive sampling

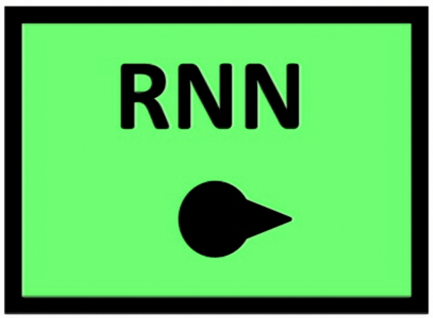


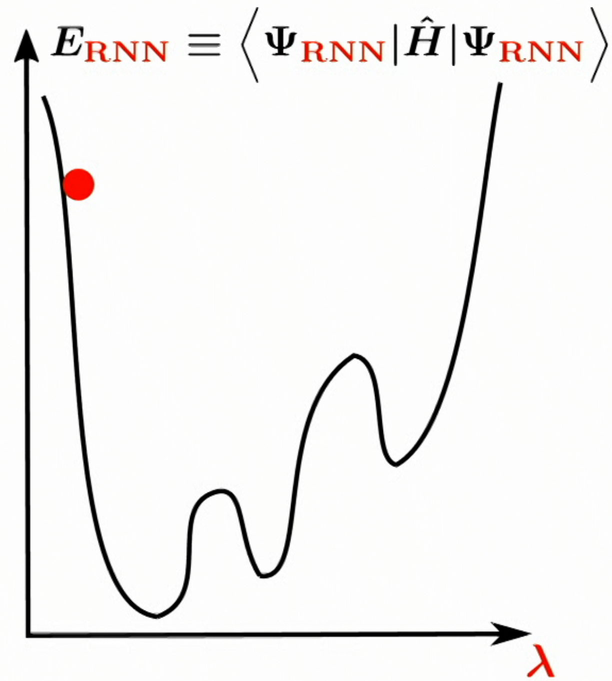
The RNN can sample from multiple modes

(very helpful in switching between topological sectors)

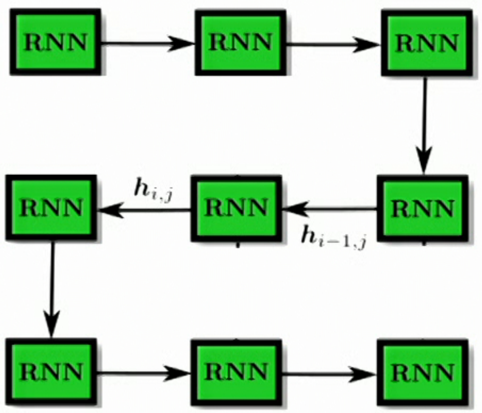
$$|\Psi_{\mathbf{RNN}}(\sigma_1, \sigma_2, \sigma_3, \sigma_4)|^2 = P(\sigma_1)P(\sigma_2|\sigma_1)P(\sigma_3|\sigma_2, \sigma_1)P(\sigma_4|\sigma_3, \sigma_2, \sigma_1)$$

RNN wave functions optimization





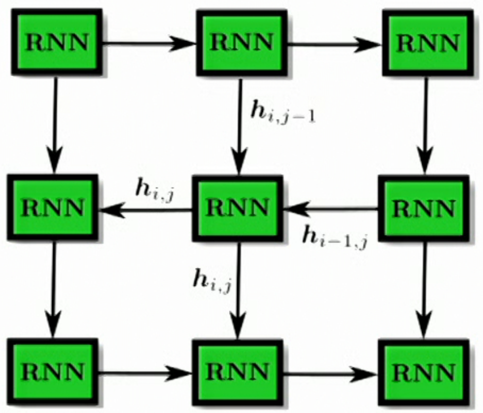
Using 1D RNNs to study 2D systems



1D recursion relation:

$$\boldsymbol{h}_n = f(W[\boldsymbol{h}_{n-1}; \boldsymbol{\sigma}_{n-1}] + \boldsymbol{b})$$

2D RNNs



~~**1D recursion relation:**~~

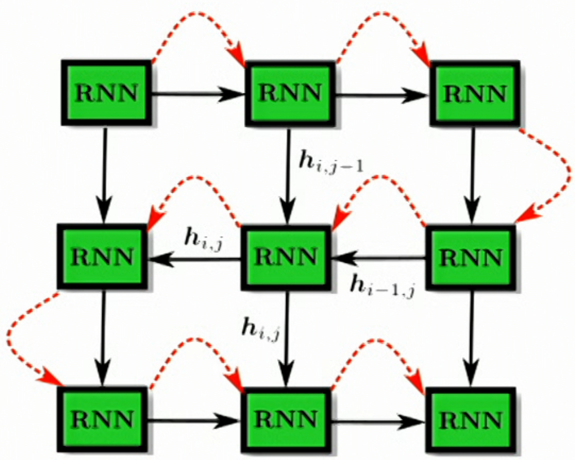
$$h_n = f(W[h_{n-1}; \sigma_{n-1}] + b)$$

2D recursion relation:

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

M.H, M. Ganahl, L. Hayward, R. Melko, J. Carrasquilla, RNN Wave functions, PRReasearch, 2020.
A. Graves, S. Fernandez, J. Schmidhuber, Multi-dimensional recurrent neural networks, 2007.
A. Graves, PhD Thesis, 2012.

Zigzag autoregressive sampling



M.H, M. Ganahl, L. Hayward, R. Melko, J. Carrasquilla, RNN Wave functions, PRReasearch, 2020.
A. Graves, S. Fernandez, J. Schmidhuber, Multi-dimensional recurrent neural networks, 2007.
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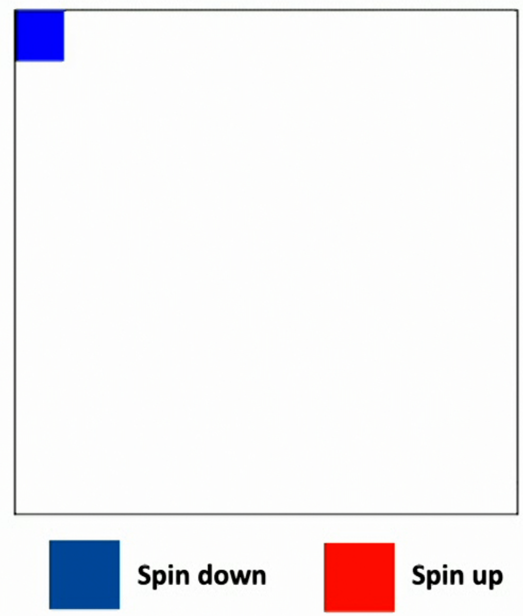
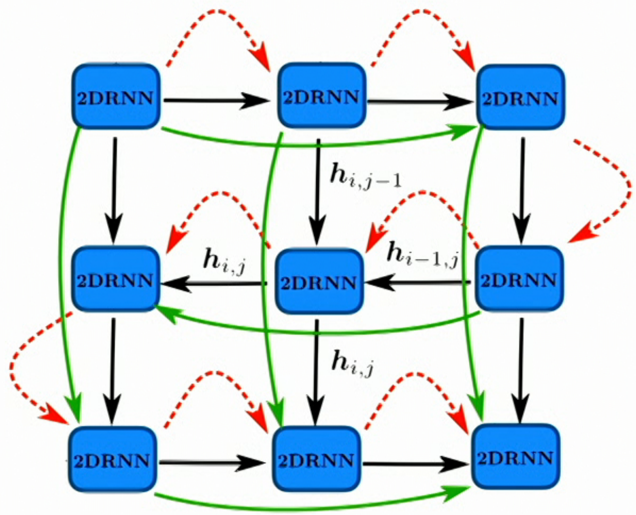


2D periodic RNNs



Adding extra connections to model periodic boundary conditions.

M.H, R. Melko, J. Carrasquilla, arXiv:2303.11207, 2023
D Luo, Z Chen, K Hu, Z Zhao, VM Hur, BK Clark, Physical Review Research 5 (1), 013216, 2023

2 - Topological order

Topological entanglement entropy

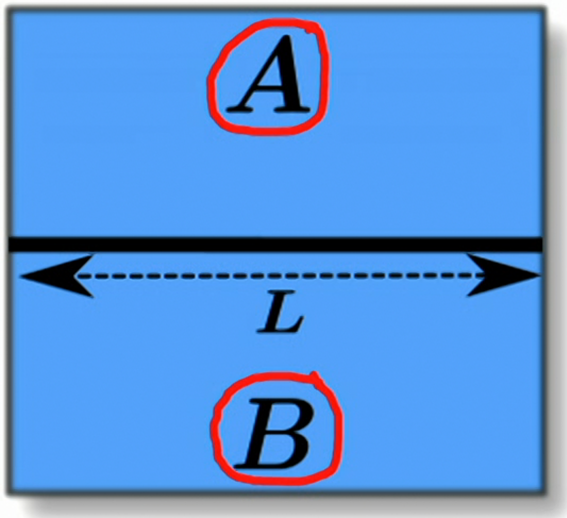
$$S_2(A) = -\log(\mathrm{Tr}(\rho_A^2))$$

Second Renyi entropy can be computed using RNN wave functions with the Swap trick.

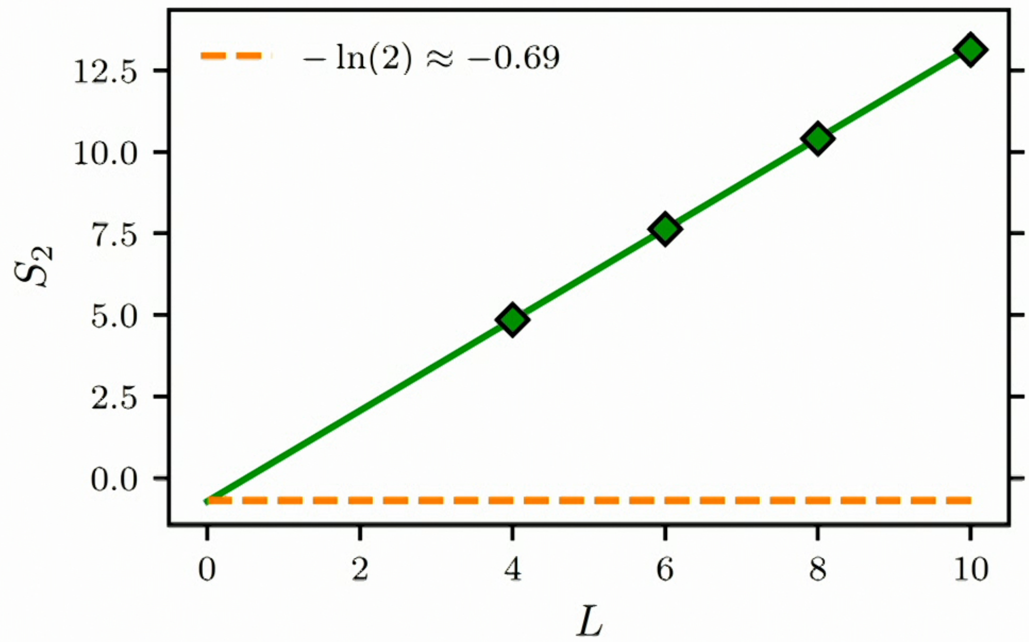
M.H, M. Ganahl, L. Hayward, R. Melko, J. Carrasquilla, RNN wave functions, PRResearch, 2020

$$S_2(A) = aL - \gamma + \mathcal{O}(L^{-1})$$

S T. Flammia, A. Hamma, T L. Hughes, XG Wen, Phys. Rev. Lett. 103, 261601 (2009)



Finite-size scaling $S_2(A) = aL - \gamma + \mathcal{O}(L^{-1})$



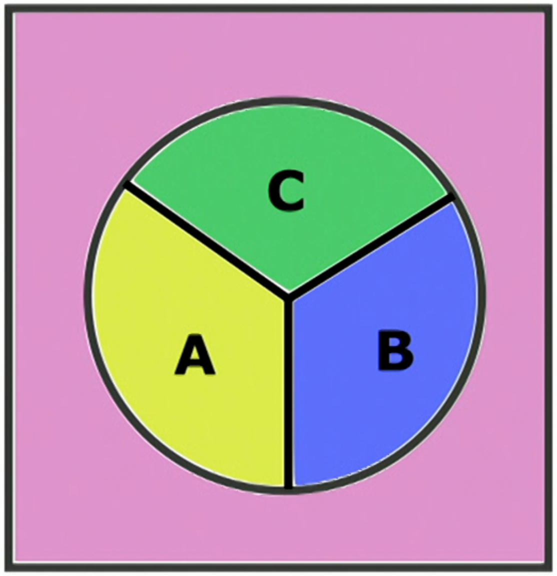
Kitaev-Preskill construction

$$\gamma = -S_A - S_B - S_C$$

$$+S_{AB} + S_{AC} + S_{BC}$$

$$-S_{ABC}$$

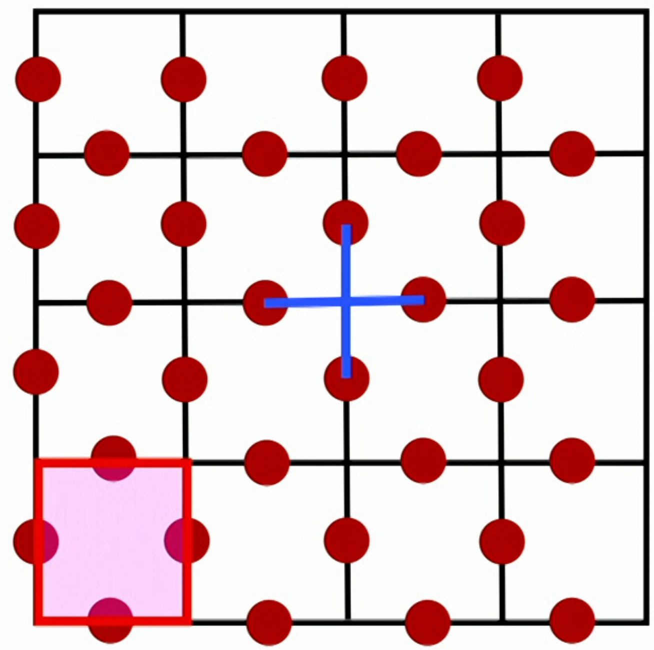
Kitaev, Preskill, 2005



3. Practical results on prototypical quantum models

2D Toric Code

$$\hat{H} = -\sum_p \Pi_{i\in p}\hat{\sigma}_i^z - \sum_v \Pi_{i\in v}\hat{\sigma}_i^x$$

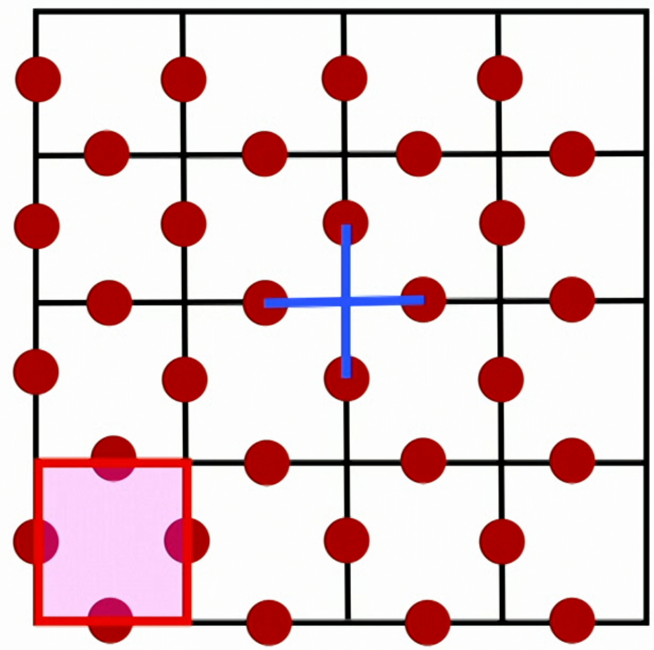


2D Toric Code

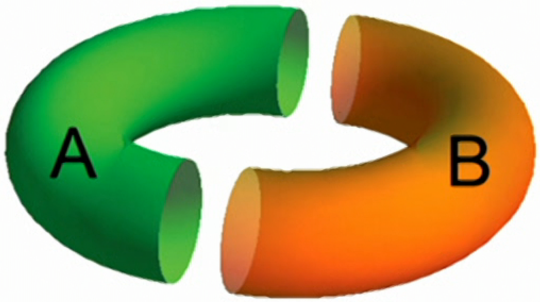
$$\hat{H} = -\sum_{p} \Pi_{i \in p} \hat{\sigma}_i^z - \sum_{v} \Pi_{i \in v} \hat{\sigma}_i^x$$

$$\gamma = \ln(2)$$

Z_2 topological order



Topological entanglement entropy in a torus

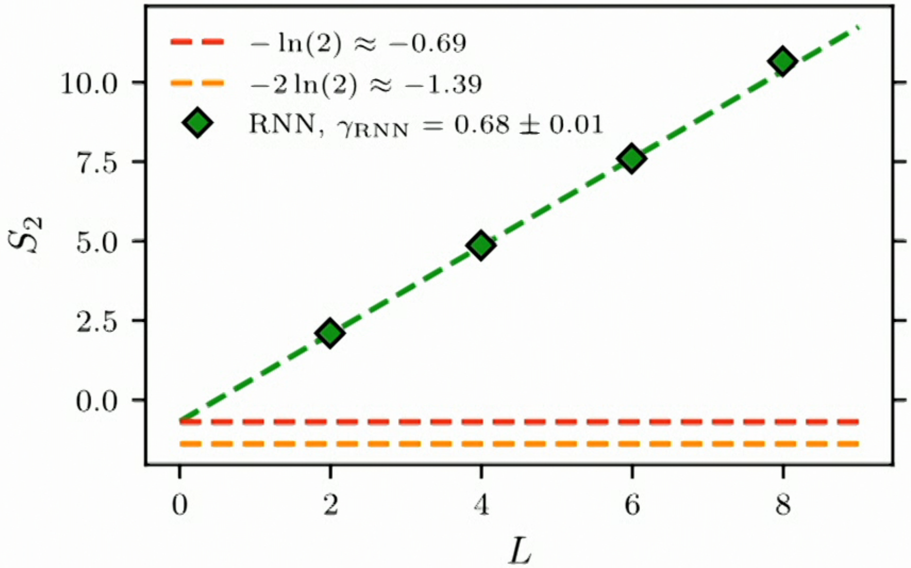


Credit: Y. Zhang, T. Grover, A. Turner, M. Oshikawa, A. Vishwanath Phys. Rev. B 85, 235151

Each cut contributes with ln(2) to the topological entanglement entropy

$$2\gamma = 2\ln(2)$$

2D Toric Code



Entanglement entropy (EE) scaling with system size

The 2D RNN can support an area law in 2D.

The 2D RNN does not find 2ln(2) but instead ln(2) for the TEE.

M.H, R. Melko, J. Carrasquilla, arXiv:2303.11207

Superposition of topological sectors

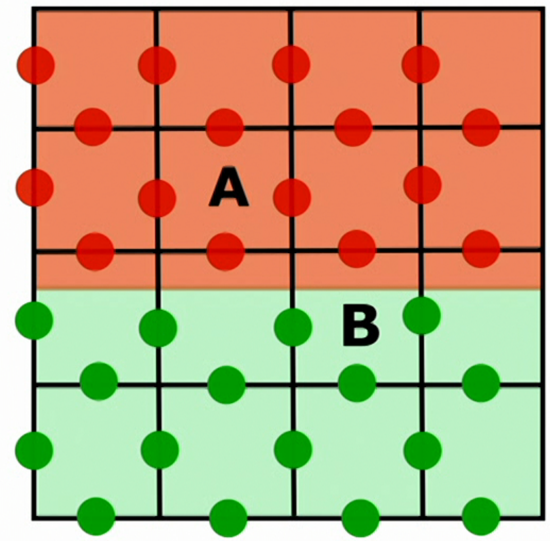
The regions we choose are **non-contractible**.

$$\gamma' = 2\gamma + \ln\left(\sum_i p_i^2\right)$$

The **TEE** becomes dependent on the **topological sector superposition**.

$$p_i = |\alpha_i|^2 \qquad |\Psi\rangle = \sum_i \alpha_i |\Xi_i\rangle$$

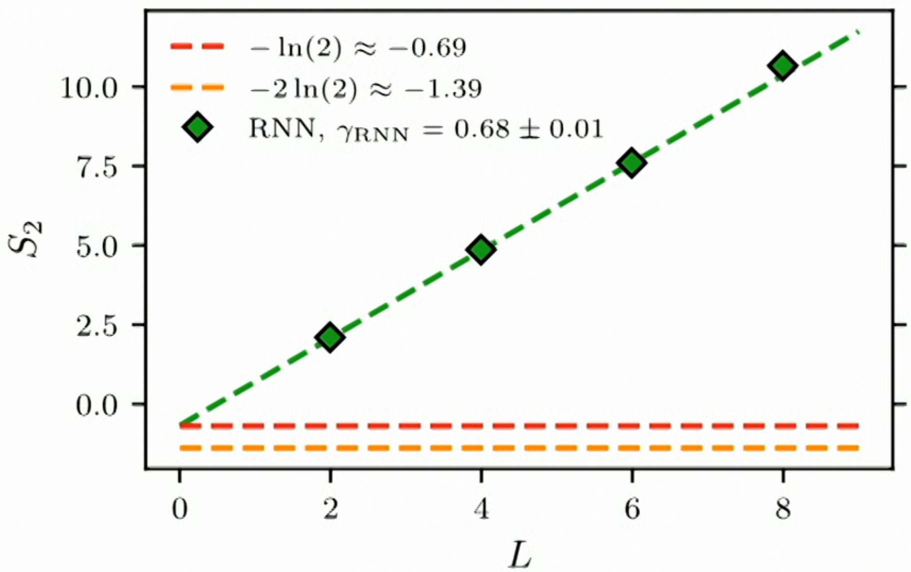
Minimally-entangled state



Cutting the torus into two cylinders

Y. Zhang, T. Grover, A. Turner, M. Oshikawa, A. Vishwanath, Phys. Rev. B 85, 235151, 2012

2D Toric Code



Entanglement entropy (EE) scaling with system size

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M.H, R. Melko, J. Carrasquilla, arXiv:2303.11207

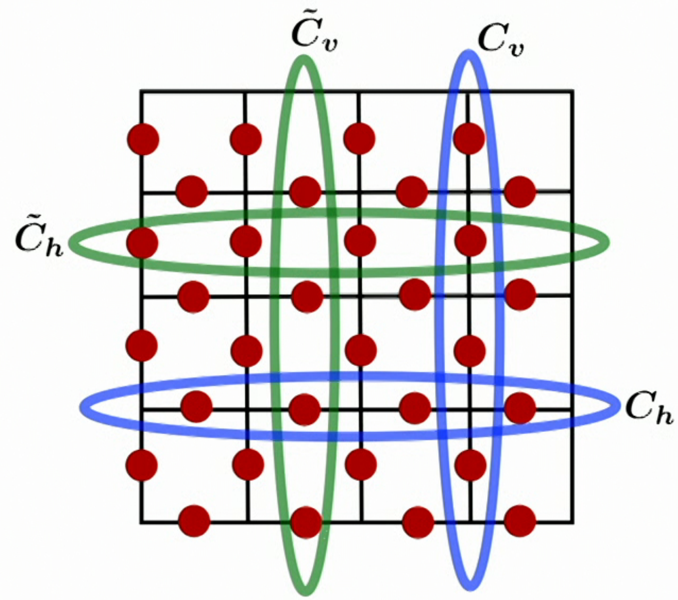
Analysis of Wilson and ‘t Hooft loops

Wilson loops of the converged **RNN wave function:**

$$\langle \hat{W}^z \rangle \approx 0$$

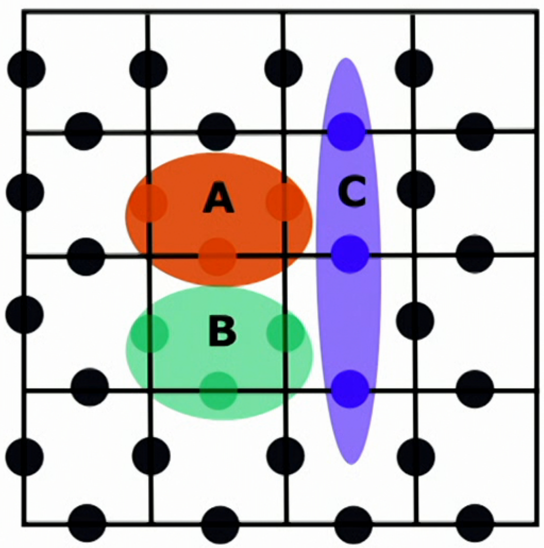
‘t Hooft loops of the converged **RNN wave function:**

$$\langle \hat{W}^x \rangle \approx +1$$

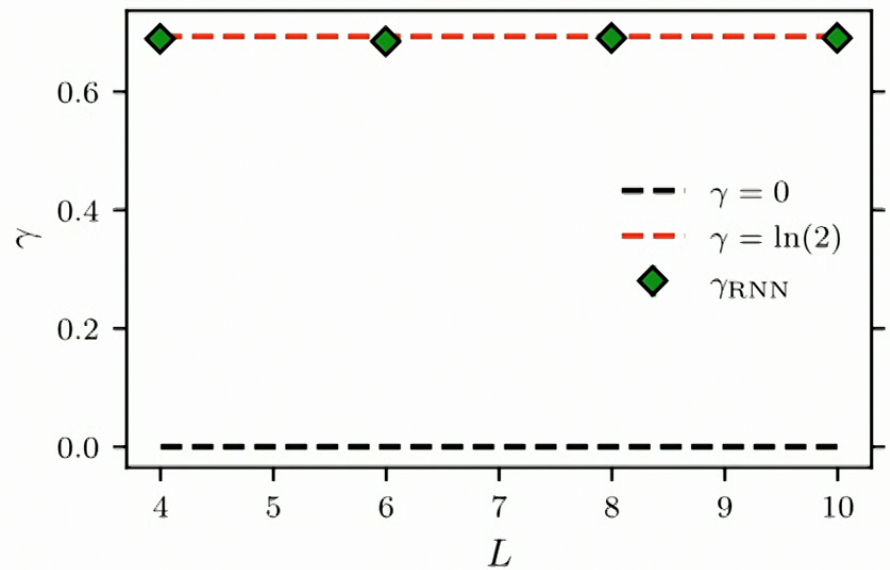


M.H, R. Melko, J. Carrasquilla, arXiv:2303.11207

2D Toric Code



The regions **A**, **B** and **C** are **contractible**.



Topological EE computed using Kitaev-Preskill construction

The **TEE** is independent of the **topological sector superposition**

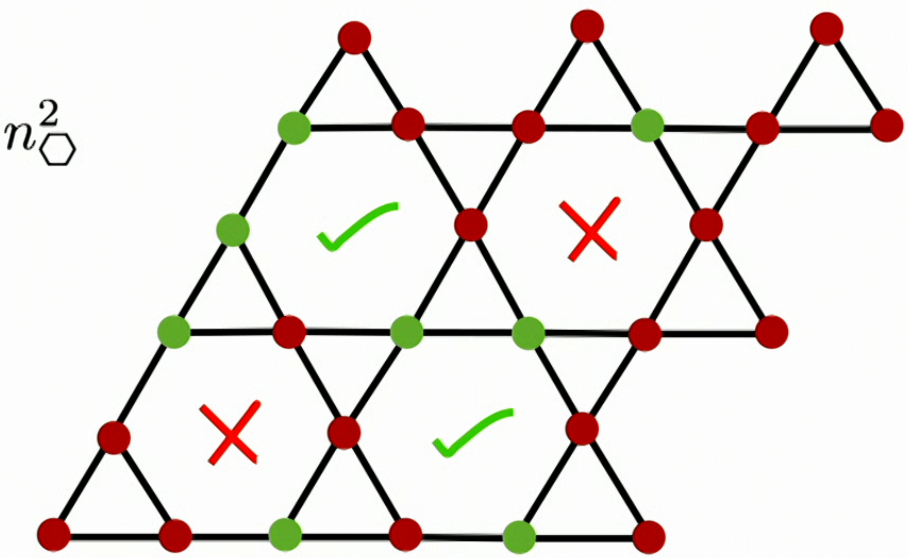
M.H, R. Melko, J. Carrasquilla, arXiv:2303.11207

Bose-Hubbard model on Kagome lattice

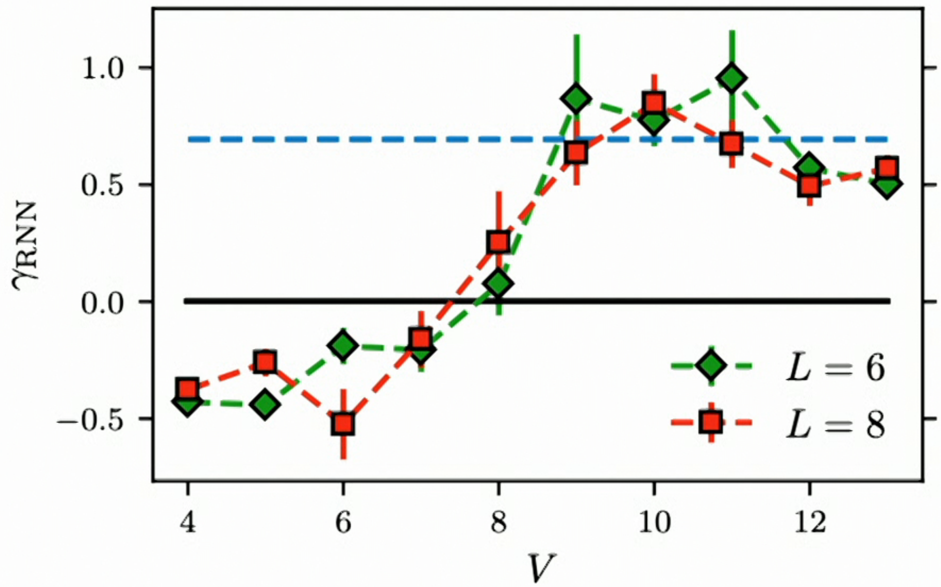
$$\hat{H} = -\sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + b_i b_j^\dagger \right) + V \sum_{\hexagon} n_{\hexagon}^2$$

$$n_{\hexagon} = \sum_{i \in \hexagon} (n_i - 1/2)$$

We use hard-core Bosons: one or zero occupation.



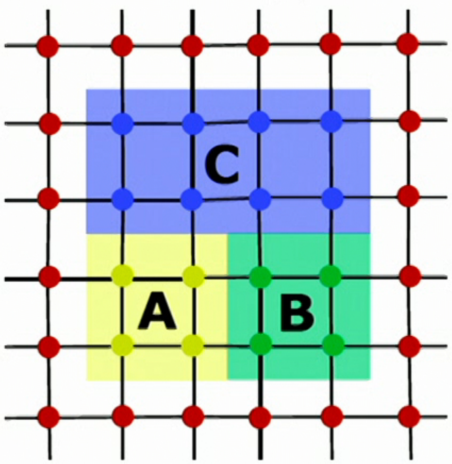
Bose-Hubbard model on Kagome lattice



Using Kitaev-Preskill construction

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

Agreement with $\ln(2)$ for large V



M.H, R. Melko, J. Carrasquilla, arXiv:2303.11207

Takeaways

- **RNN wave functions** **can be used to calculate** **topological entanglement entropies** **to detect** **topological order**.
- **RNN wave functions** **finds superpositions of** **minimally-entangled states**.
- **RNN wave functions** **can numerically support** **area law** **scaling of** **entanglement entropy.**

Future directions

- Using RNN wave functions to investigate topological properties of real-world quantum systems namely Rydberg atoms arrays and trapped ions using Variational Monte Carlo/quantum state tomography.

Thank you for your attention!

- RNN wave functions can be used to calculate topological entanglement entropies to detect topological order.
- RNN wave functions finds superpositions of minimally-entangled states.
- RNN wave functions can numerically support area law scaling of entanglement entropy.