Title: Learning the sign structures of quantum systems: is it hard or trivial?

Speakers: Tom Westerhout

Series: Machine Learning Initiative

Date: December 02, 2022 - 2:00 PM

URL: https://pirsa.org/22120021

Abstract: A well-established approach to solving interacting quantum systems is variational Monte Carlo. There is a lot of renewed interest in it since the introduction of neural networks as a highly expressive and unbiased variational ansatz. Similar to more traditional ansätze, neural networks struggle with solving frustrated quantum systems. A conjecture has been made that the cause of these difficulties lies in the sign structures of the ground state wavefunctions. Here, we will discuss these sign structures in more detail and try to analyze how complex they really are by establishing a connection to classical Ising models.

Zoom link: https://pitp.zoom.us/j/99087954160?pwd=Vm5zWWRFbHBwVFR1RHZMc3ptem03QT09

Learning the sign structures of quantum systems: is it hard or trivial?

Tom Westerhout
Theory of Condensed Matter
Radboud University

2 December

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Acknowledgements

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Radboud University

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Andrey A. Bagrov

Skoltech
Skolkovo Institute of Science and Technology

Konstantin S. Tikhonov

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Radboud University

Radboud University

- Located in Nijmegen — the oldest city in the Netherlands;
- In 2010 Andre Geim and Konstantin Novoselov got a Nobel Prize in Physics for the discovery of graphene;

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Theory of Condensed Matter

- Electronic structure calculations
- Plasmonics
- Superconductivity
- Spintronics
- Statistical physics of membranes
- Quantum mechanics on fractals
- Quantum many-body theory
- Complexity

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Complexity

- Structural complexity

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Complexity

- Structural complexity
- Biological complexity
- Complexity in quantum systems

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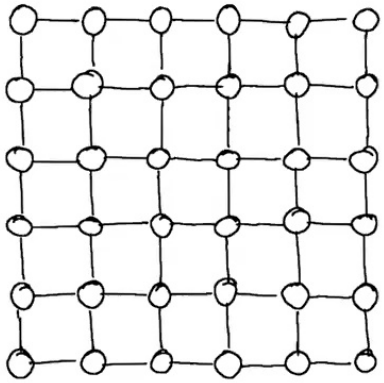
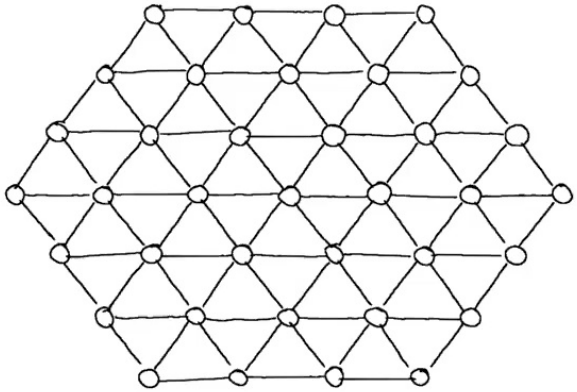
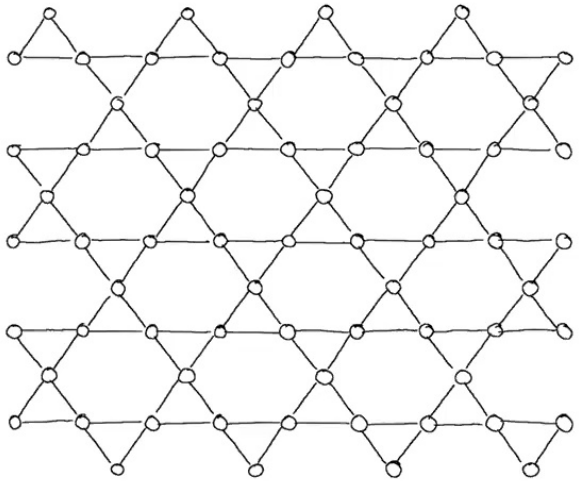
Complexity in quantum systems



Simple



Meh...



Difficult

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Plan

Stick to simple objects — ground states.

- Ground states of frustrated magnets are difficult to learn.
- It's the sign structure that's difficult, not the amplitudes.
- Alternative formalism to describe the sign structures.
- In this formalism, even frustrated magnets don't seem very difficult.

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Part 1

ARTICLE

https://doi.org/10.1038/s41467-020-15402-w OPEN

Check for updates

Generalization properties of neural network approximations to frustrated magnet ground states

Tom Westerhout[1✉], Nikita Astrakhantsev[2,3,4✉], Konstantin S. Tikhonov[5,6,7✉], Mikhail I. Katsnelson[1,8] & Andrey A. Bagrov[1,8,9✉]

NATURE COMMUNICATIONS, 11(1), 1-8. DOI:10.1038/S41467-020-15402-W

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Learning

- Exact diagonalization can treat systems of up to 48-50 spins [1].
- Can't save (or *remember*) everything.
- Need to *learn* it.
- Neural networks are good at learning.

[1] PHYSICAL REVIEW E, 98(3), 033309. DOI:10.1103/PHYSREVE.98.033309

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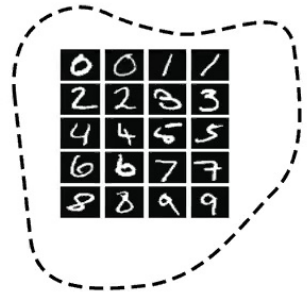
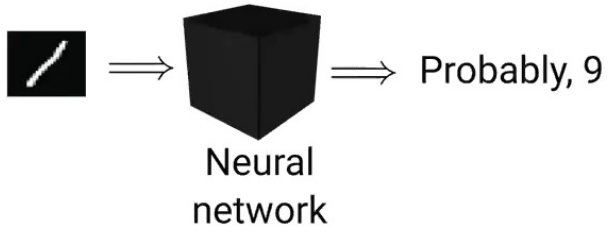
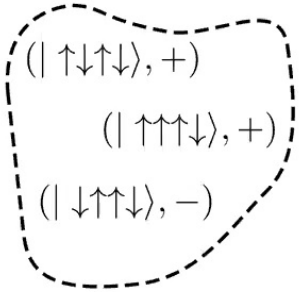
Supervised learning

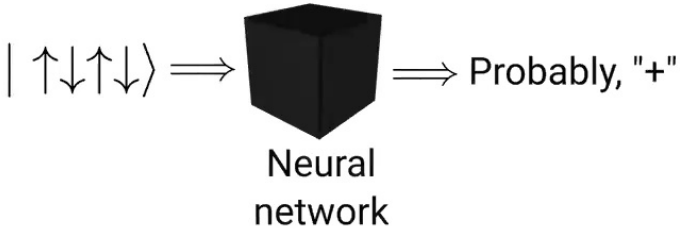


MNIST dataset





Ground state



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Hamiltonians

Stick to simple models: ~~Ising in transverse field~~ Heisenberg model

$$H = J_1 \sum_{\langle a,b \rangle} \hat{\boldsymbol{\sigma}}_a \otimes \hat{\boldsymbol{\sigma}}_b + J_2 \sum_{\langle\langle a,b \rangle\rangle} \hat{\boldsymbol{\sigma}}_a \otimes \hat{\boldsymbol{\sigma}}_b$$

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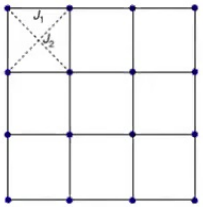
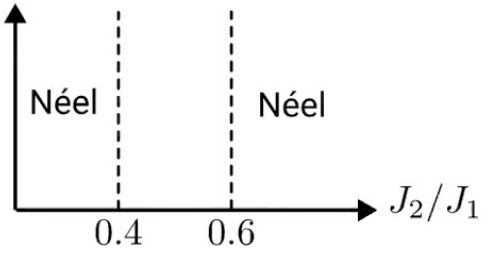
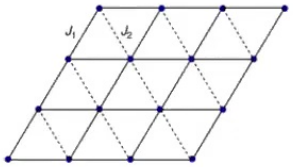
Systems

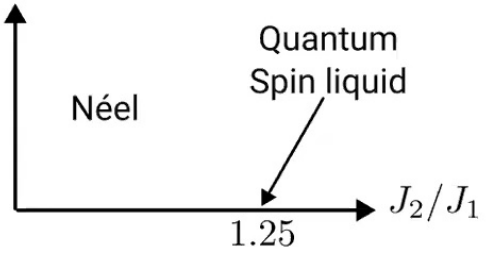
Square lattice



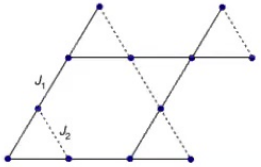


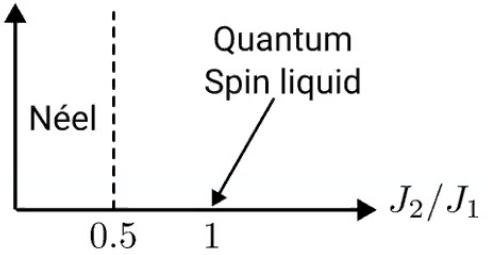
Triangular lattice





Kagome lattice





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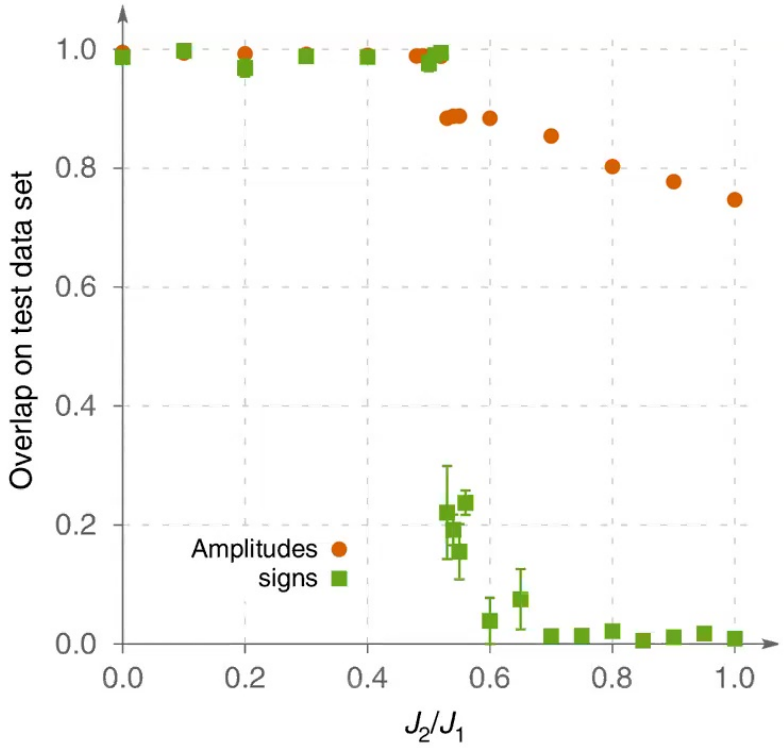
Amplitudes vs Signs



- 24 site Kagome lattice;
- Trained on $2.7 \cdot 10^4$ out of $2.7 \cdot 10^6$ basis vectors (i.e. 1%);

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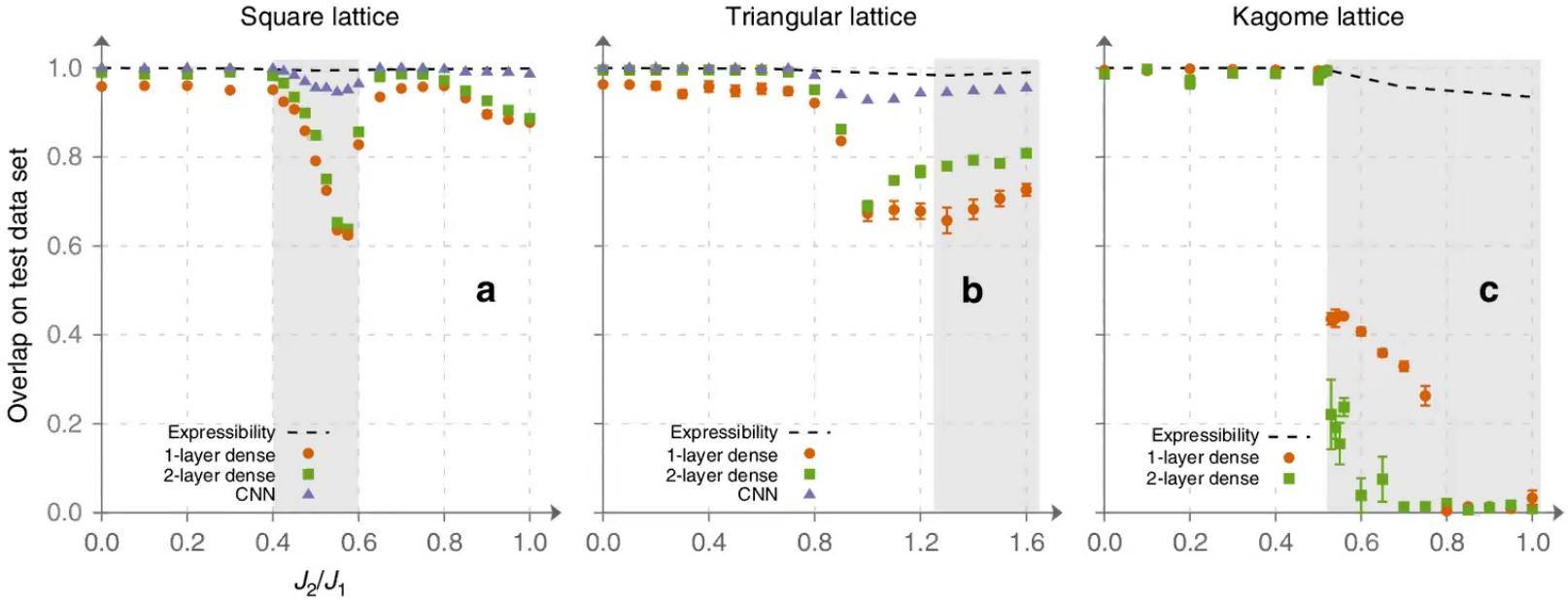
Sign structure generalization



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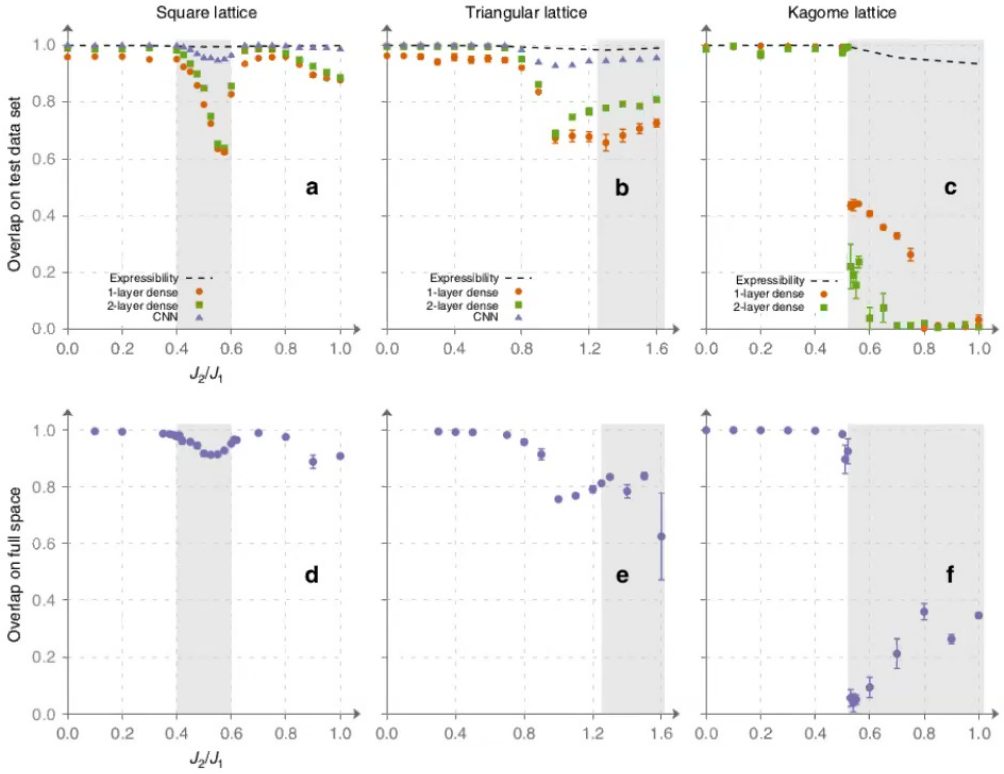
Recap

- Signs are more difficult to learn than amplitudes;
- This difficulty is correlated with frustration;

Relation to real VMC simulations?



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Fun facts

- Y. Nomura and M. Imada in [1]:
  0.01% error for the 6x6 **square** lattice in the QSL and VBS phases.
- C. Roth, Attila Szabó, and A. H. MacDonald in [2]:
  0.05% error for the 6x6 **triangular** lattice in the QSL phase.
- D. Kochkov, T. Pfaff, A. Sanchez-Gonzalez, P. Battaglia, and B.K. Clark in [3]:
  1-2% error for the 36-site **Kagome** lattice in the QSL phase
  (and overlap is just 60%).

[1] PHYSICAL REVIEW X, 11(3), 031034. DOI:10.1103/PHYSREVX.11.031034

[2] ARXIV:2211.07749.

[3] ARXIV:2110.06390.

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What to do with the Kagome lattice

Use mVMC 😄

COMPUTER PHYSICS COMMUNICATIONS, 235, 447-462. 10.1016/J.CPC.2018.08.014

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Part 2

Unveiling ground state sign structures of frustrated quantum systems via non-glassy Ising models

Tom Westerhout,[1,*] Mikhail I. Katsnelson,[1,†] and Andrey A. Bagrov[1,‡]

[1] *Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525AJ Nijmegen, The Netherlands*

- Alternative formalism to describe the sign structures.
- In this formalism, even frustrated magnets don't seem very difficult.

ARXIV:2207.10675.

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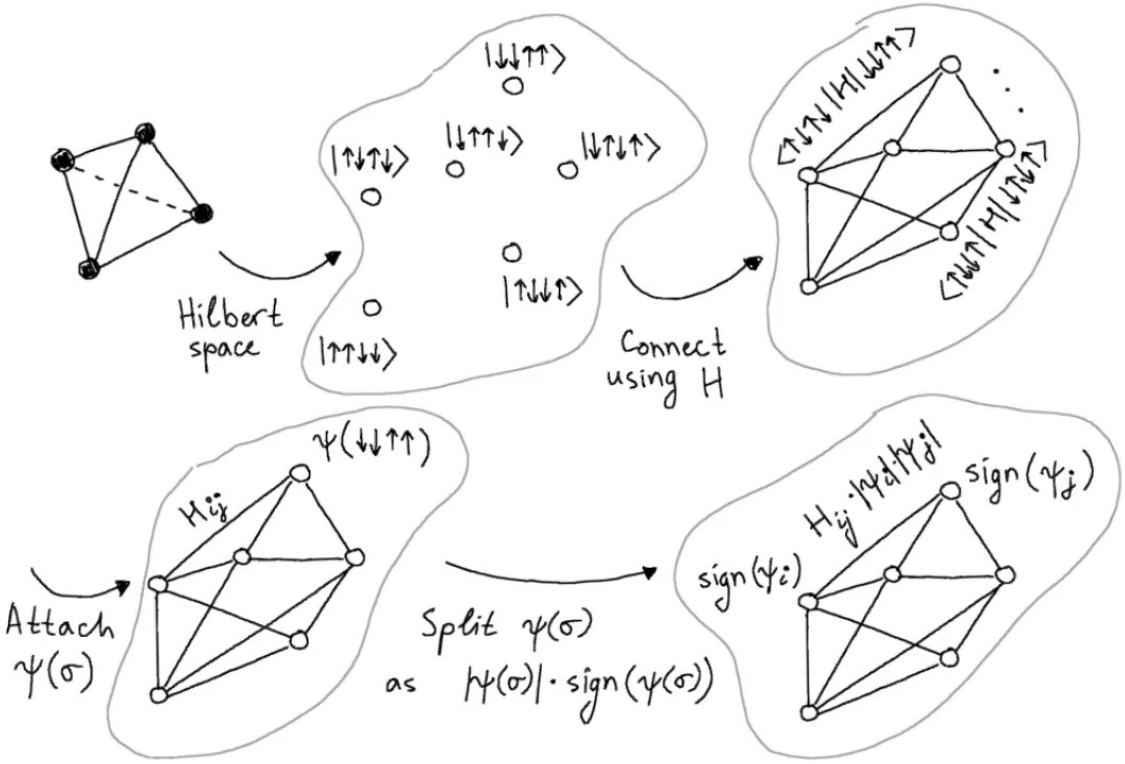
Hilbert spaces and Ising models



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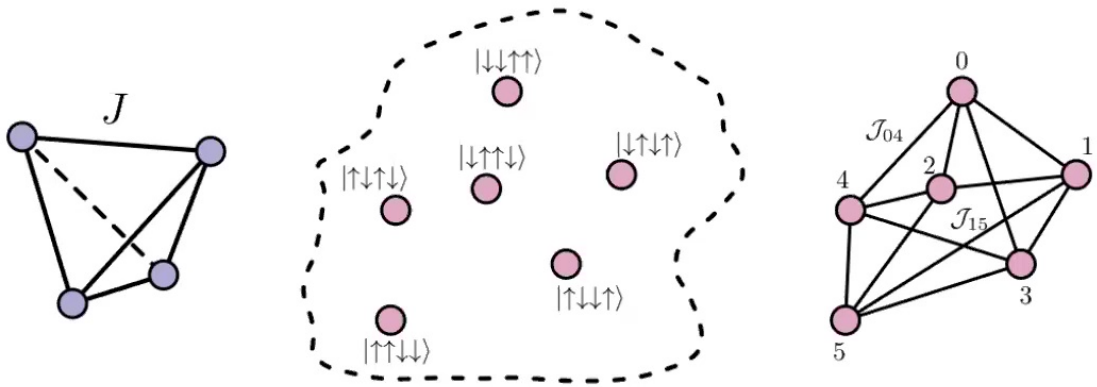
More formally



Real lattice Hilbert space Ising model

$$|\psi\rangle = \sum_i \psi_i |i\rangle = \sum_i \mathcal{S}_i \, |\psi_i| \, |i\rangle$$

$$E = \langle\psi|H|\psi\rangle = \sum_{i,j} \langle i|H|j\rangle |\psi_i||\psi_j| \mathcal{S}_i \mathcal{S}_j = \sum_{i,j} \mathcal{J}_{i,j} \mathcal{S}_i \mathcal{S}_j$$

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Unfrustrated systems

- Heisenberg antiferromagnet on the square lattice.
- Sign structure is known — Marshall's sign rule.
- Auxiliary Ising model turns out to be unfrustrated as well!

MARSHALL, W. (1955). ANTIFERROMAGNETISM. PROCEEDINGS OF THE ROYAL SOCIETY OF LONDON. SERIES A. MATHEMATICAL AND PHYSICAL SCIENCES, 232(1188), 48-68.

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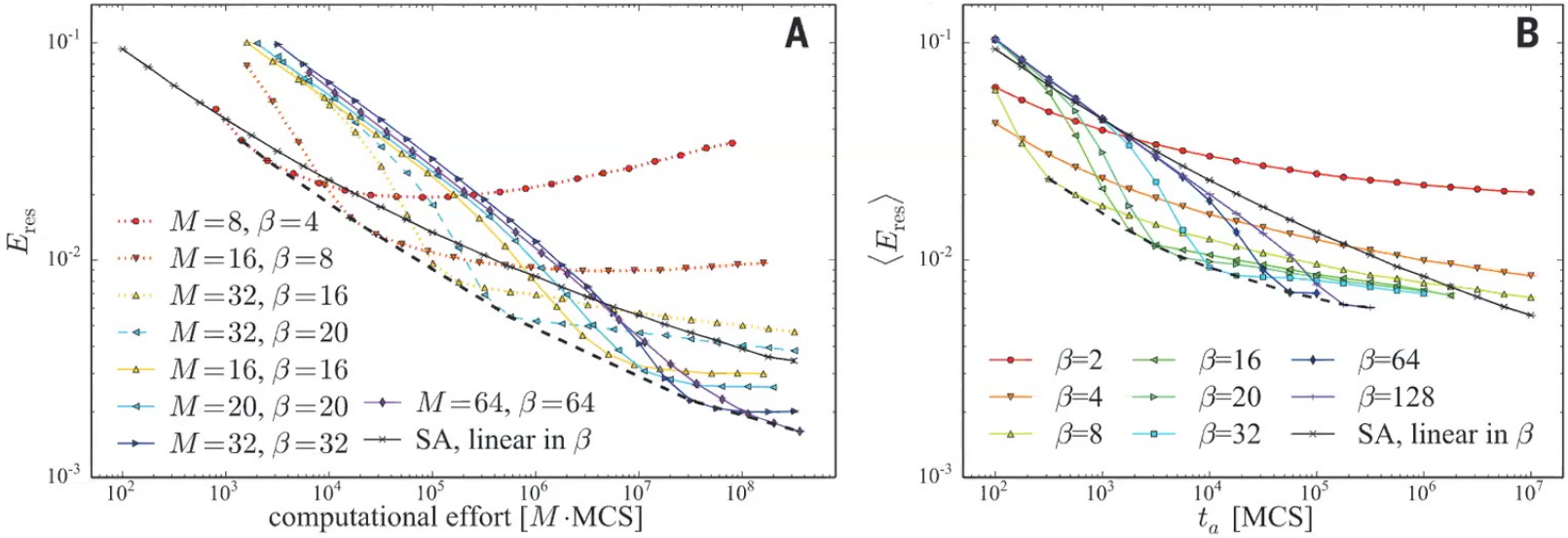
Frustrated systems

Ising model with general interactions — glassy and NP-hard ☹



SCIENCE, 348(6231), 215-217. DOI:10.1126/SCIENCE.AAA4170

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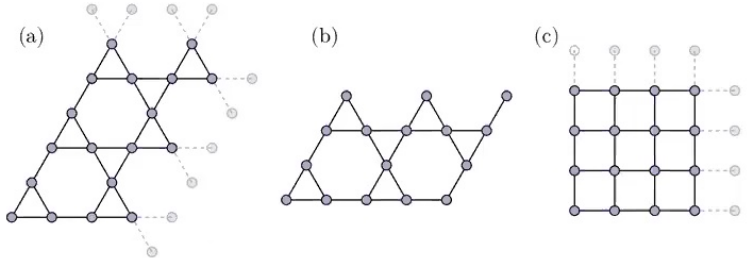
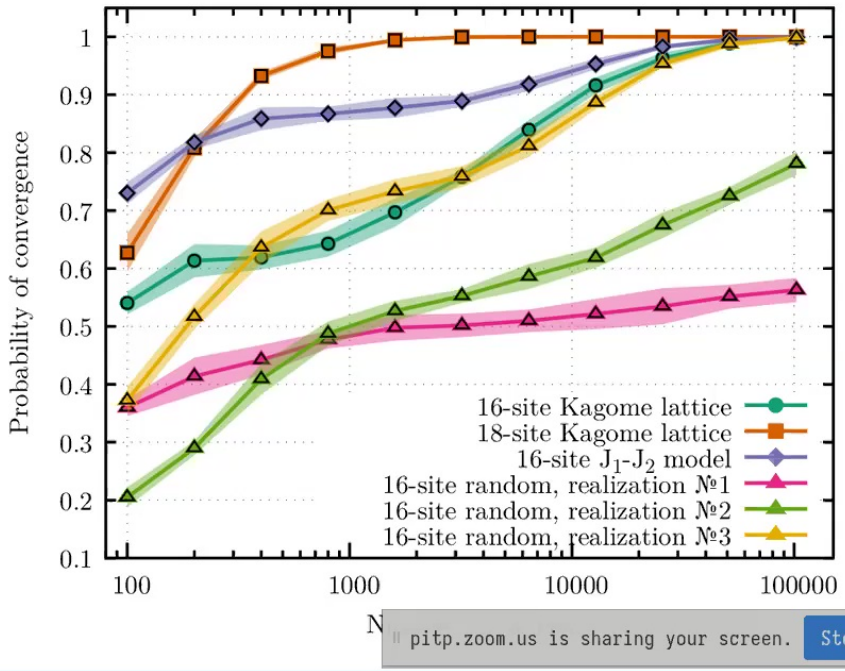
Frustrated systems





- Solutions from ED;
- Simulated Annealing (SA) on 12870 or 48620 spins;
- Converged if accuracy is at least 99.5%;

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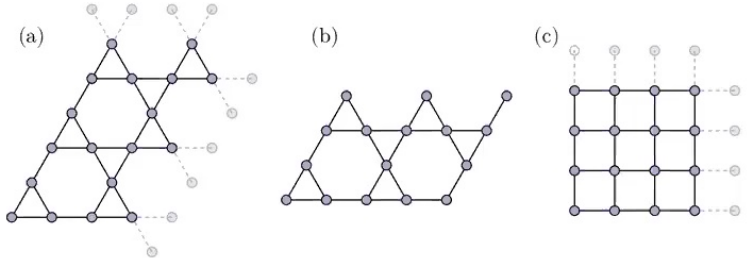
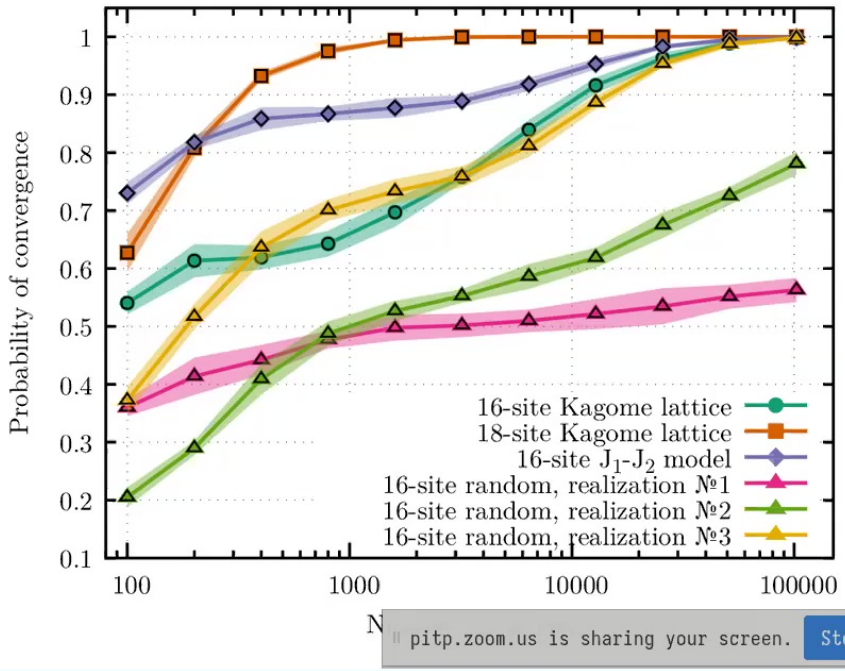
Frustrated systems





- Solutions from ED;
- Simulated Annealing (SA) on 12870 or 48620 spins;
- Converged if accuracy is at least 99.5%;
- $(1/2)^{20} \approx 10^{-6}$

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Not glassy, what now?

1. "Great, but how does it help me?"
2. "Great, but why?"

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Frustration

The system is frustrated
if "divide and conquer" approaches don't work,
i.e. local optimization doesn't work

invert

The system is mildly frustrated,
is there then hope for local optimization?

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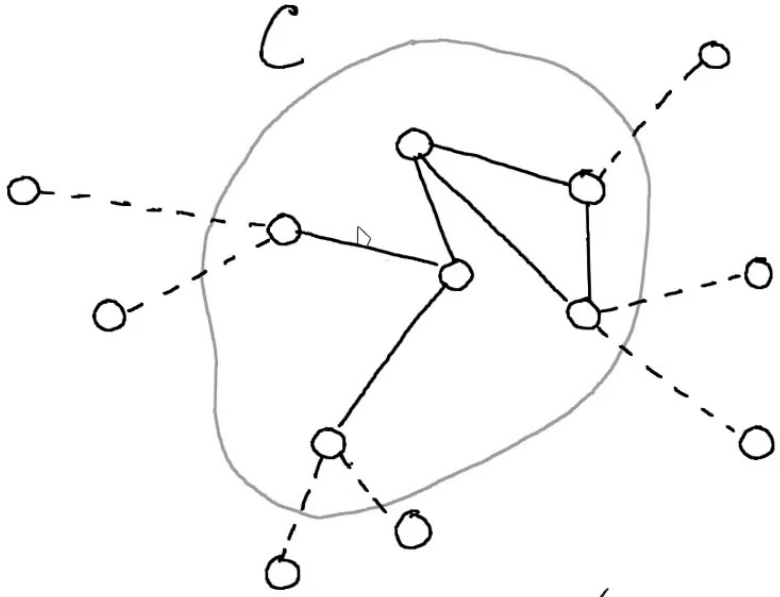
Subset of the Hilbert space



Optimize only $\mathcal{S}_i$ for $i \in \mathcal{C}$

$$H = \sum_{i,j \in \mathcal{C}} \mathcal{J}_{i,j} \mathcal{S}_i \mathcal{S}_j + \sum_{i \in \partial\mathcal{C}} \underbrace{\left(\sum_{j \notin \mathcal{C}} \mathcal{J}_{i,j} \mathcal{S}_j \right)}_{\text{Magnetic field}} \mathcal{S}_i + \sum_{i,j \notin \mathcal{C}} \mathcal{J}_{i,j} \mathcal{S}_i \mathcal{S}_j$$

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Subset of the Hilbert space

Works very well, **but**...

What about "the environment"?

We don't know it, so let's ignore it 🙄

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Subset of the Hilbert space

Works very well, **but**...

What about "the environment"?

We don't know it, so let's ignore it 🙄

Doesn't work as well

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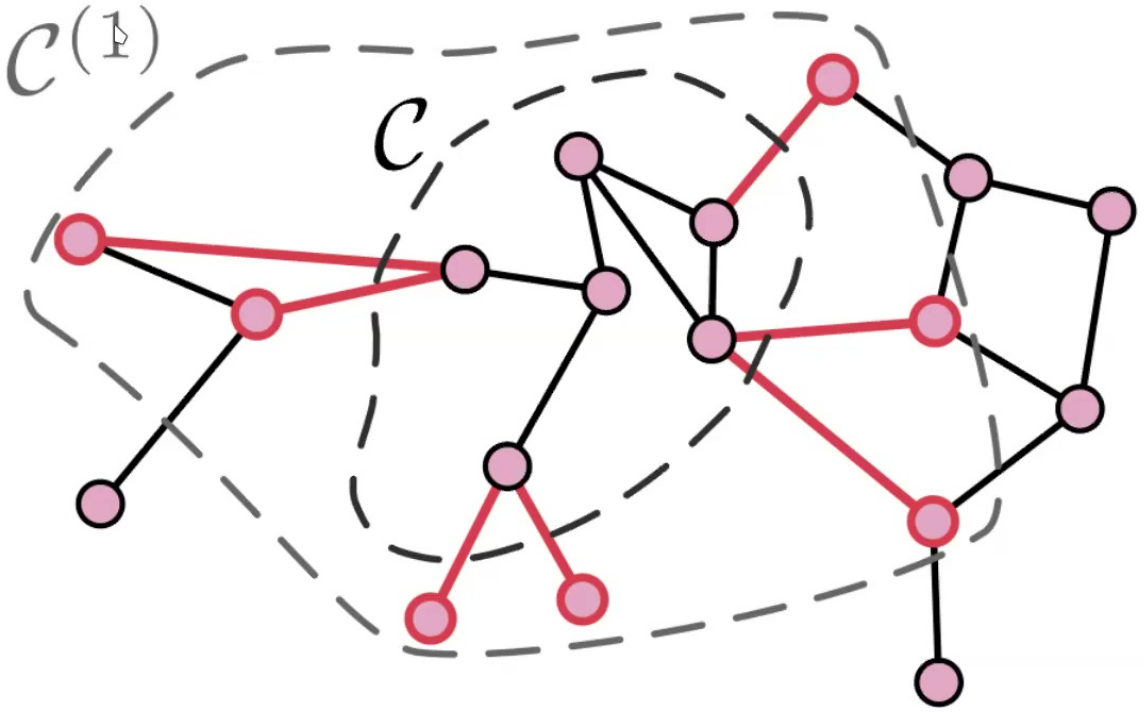
Cluster extensions



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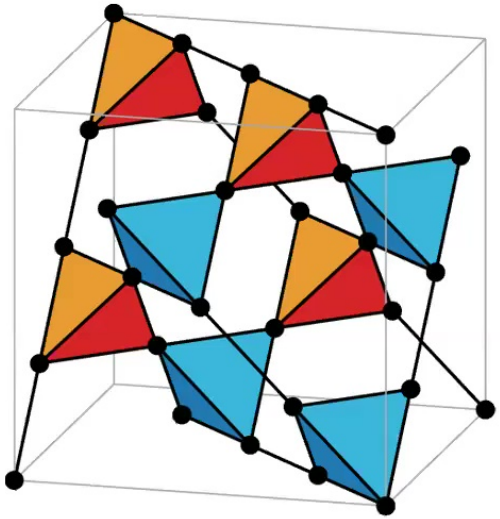
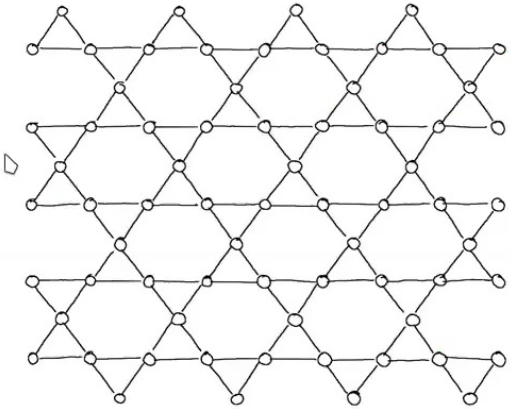
Quality metrics

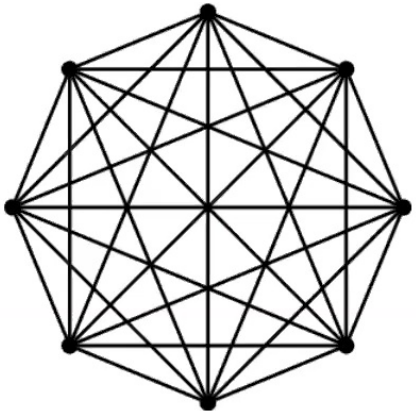
Pyrochlore lattice



Kagome lattice



Random all-to-all



$$O_{\mathcal{C}} = \frac{1}{\sum_{i\in\mathcal{C}} |\psi_i|^2} \cdot \sum_{i\in\mathcal{C}} \overbrace{|\psi_i|\mathcal{S}_i}^{\text{Variational}} \underbrace{\psi_i}_{\text{Exact}}$$

PHYSICAL REVIEW B, 84(14), 144432. 10.1103/PHYSREVB.84.144432

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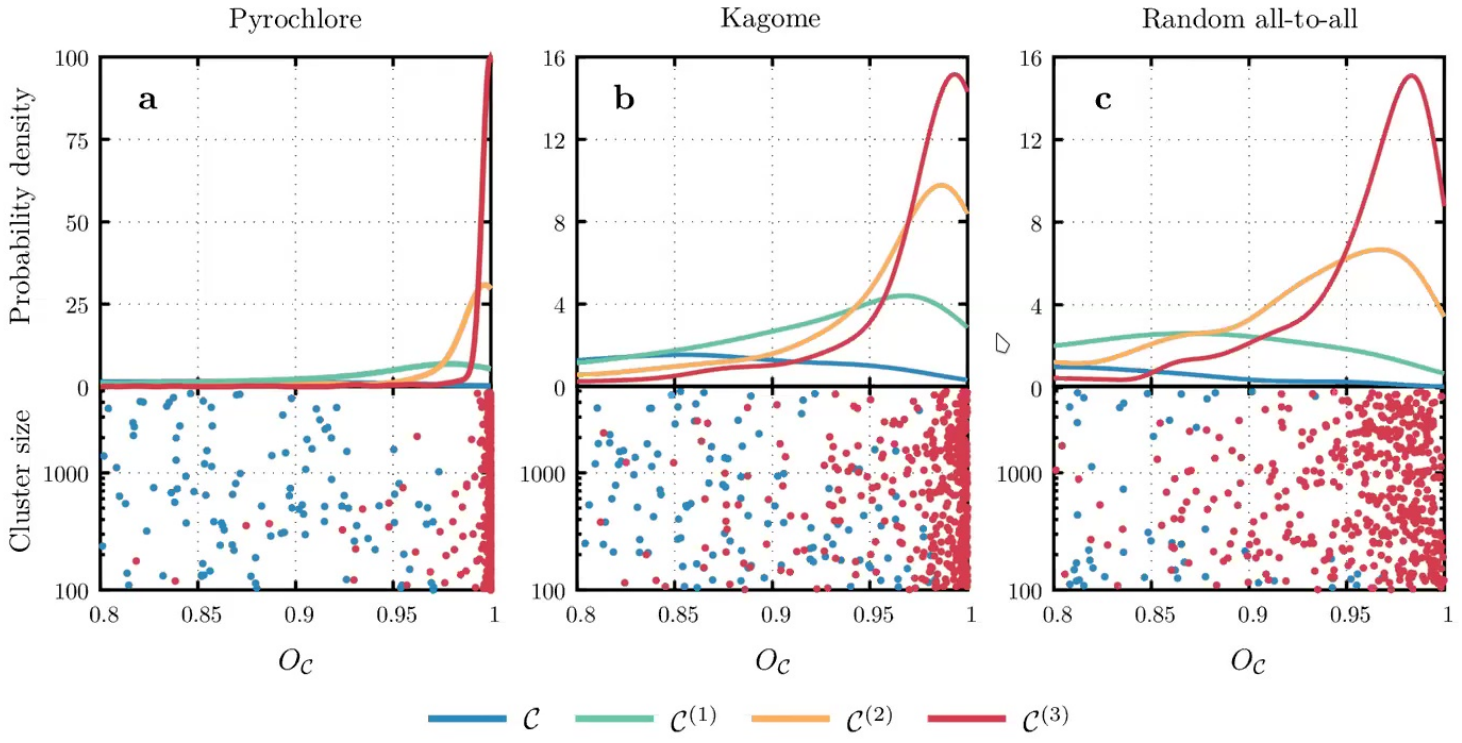
Results



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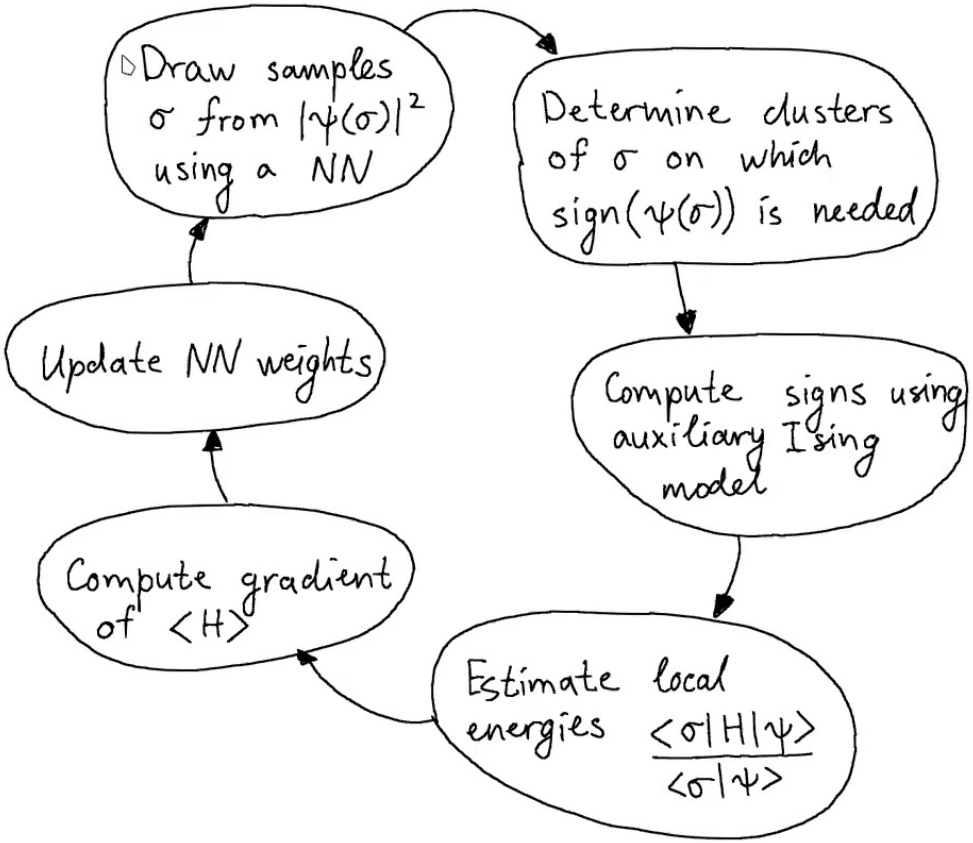
Recap

- Sign structures are not glassy, i.e. "simple".
- High-quality local optimization is possible in polynomial time, $\mathcal{O}(M \cdot N^k)$.

Potential for applications in VMC



- Robustness to noise.
- Better algorithms for building and solving $\mathcal{C}^{(k)}$.

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"Great, but why?" part

Disclaimer

The following slides contain unpublished data, take them with a grain of salt

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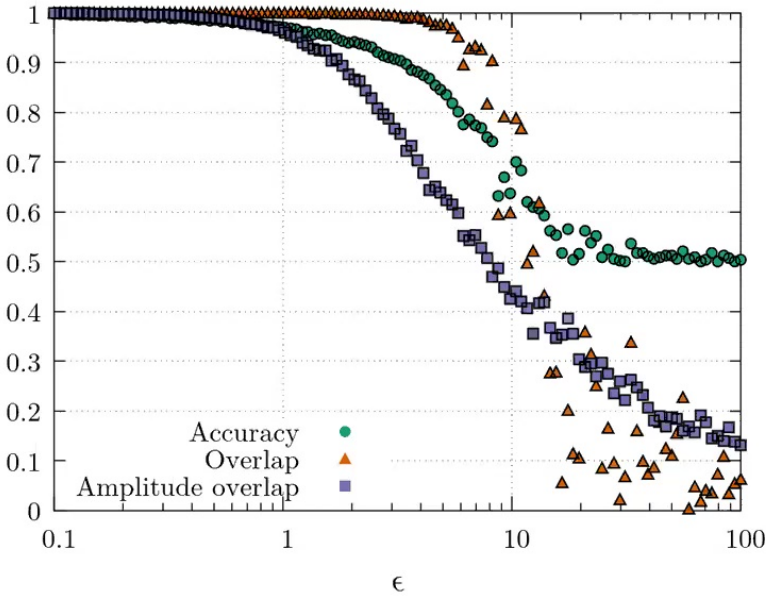
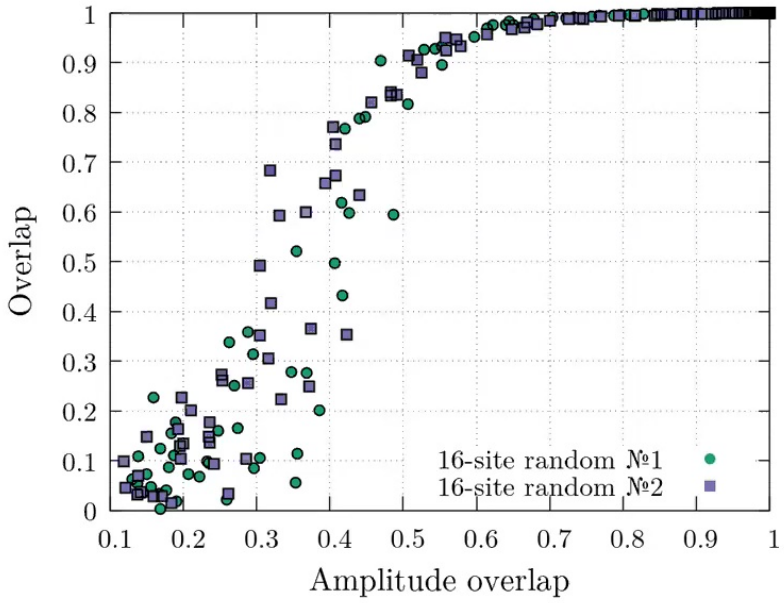
Noise in amplitudes

$$\log \psi(\sigma) \to \log \psi(\sigma) + \mathcal{U}(-\tfrac{\epsilon}{2}, \tfrac{\epsilon}{2})$$





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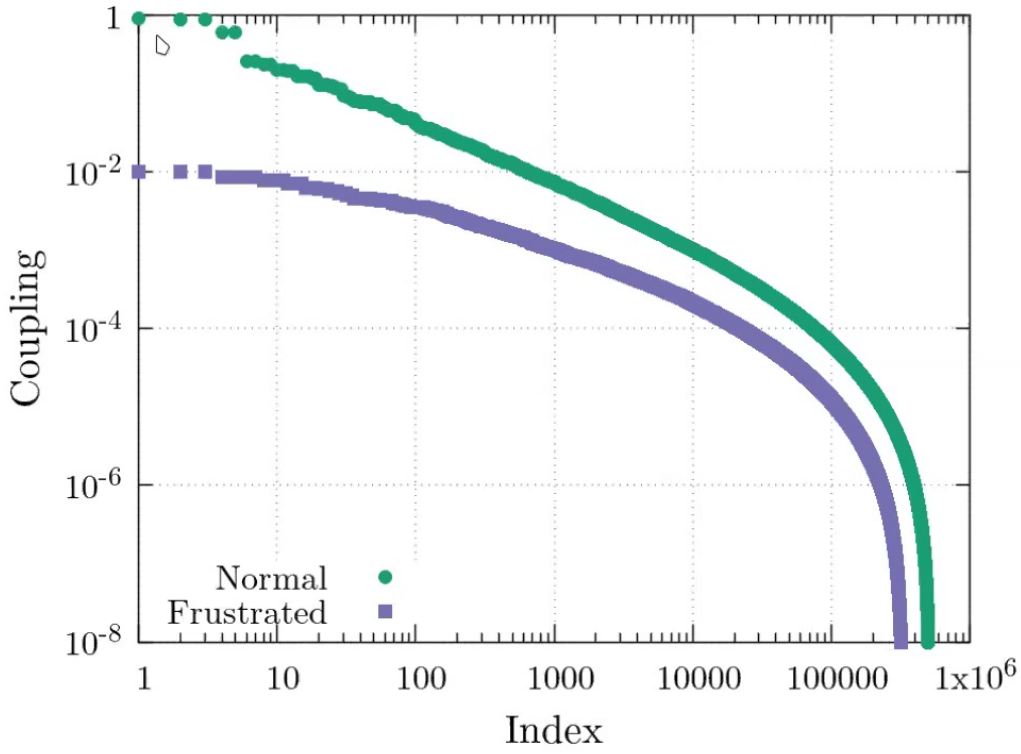
Distribution of $\mathcal{J}_{i,j}$



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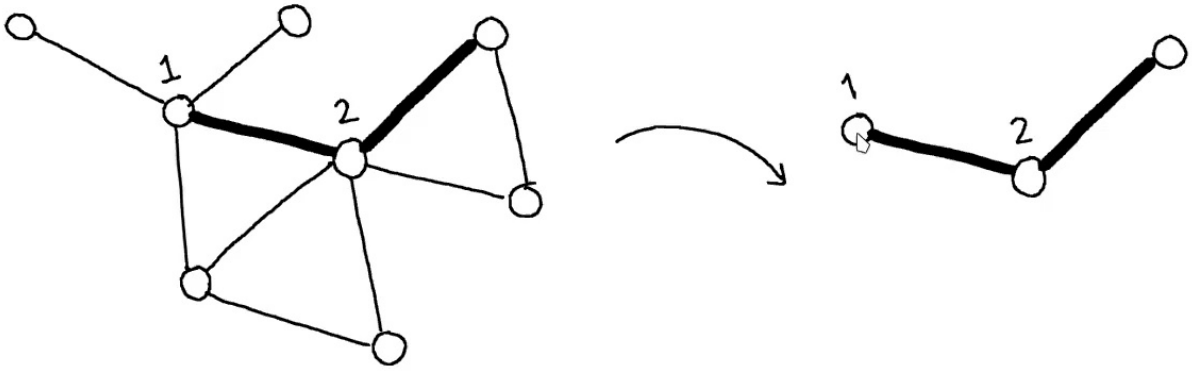
Largest couplings only



System	Accuracy	Overlap
Kagome, 16	93.4%	99.96%
Kagome, 18	90.5%	99.99%
J_1-J_2, 16	82.5%	99.5%
Random №1, 16	76.3%	98.3%
Random №2, 16	75.1%	98.2%
Random №3, 16	72.7%	96.0%

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Conclusion

- Ground states of frustrated magnets are difficult to learn.
- It's the sign structure that's difficult, not the amplitudes.
- Auxiliary Ising models as an alternative formalism for the sign structures.
- In this formalism, even frustrated magnets don't seem very difficult.

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