Title: How to solve quantum many-body problems.

Speakers: Annabelle Bohrdt

Series: Colloquium

Date: March 27, 2023 - 1:30 PM

URL: https://pirsa.org/23030116

Abstract: In quantum many-body physics, we aim to understand and predict the exciting phenomena emerging from the interactions of many quantum particles. In this talk I will use the paradigmatic Fermi-Hubbard model, a conceptually simple model of interacting fermionic particles, as an example to highlight different approaches to gain insights into quantum many-body problems. I will describe a semi-analytical theory, established numerical methods, machine learning techniques, as well as quantum simulation experiments, which provide detailed information about the quantum state of the system. A particular focus will be on how to combine these different approaches to learn as much as possible about the system of interest, for example through new observables and modified microscopic models.

Zoom link: https://pitp.zoom.us/j/94368447256?pwd=clhQcUJNaTR0UjVydnBHelo4N3JIQT09

Simple set of rules:

- avoid crowding your neighbors
- align with your neighbors
- steer towards the average position of your neighbors.

Perimeter, March 2023

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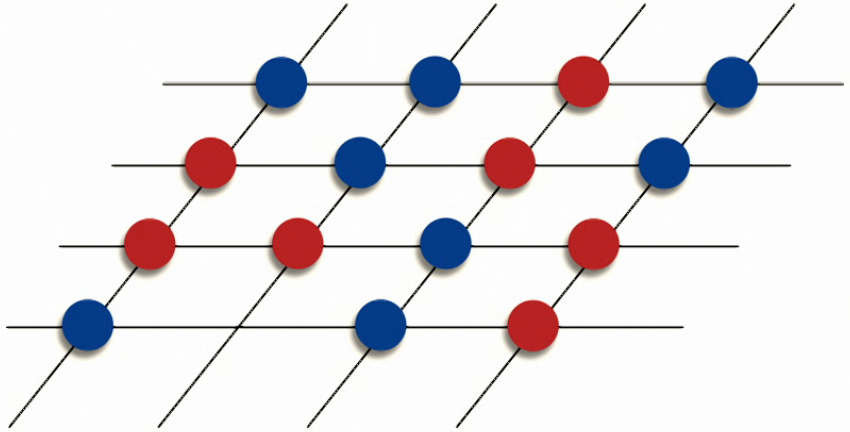
Quantum many-body systems



Simple set of rules:

- Hop around as much as possible
- Never sit on the same site as fermion with equal spin
- Try to avoid sitting on same site as fermion with opposite spin

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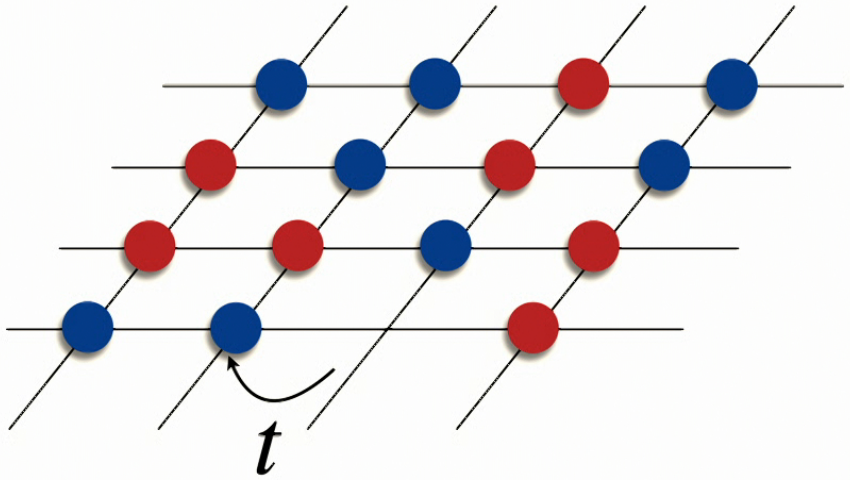
Quantum many-body systems



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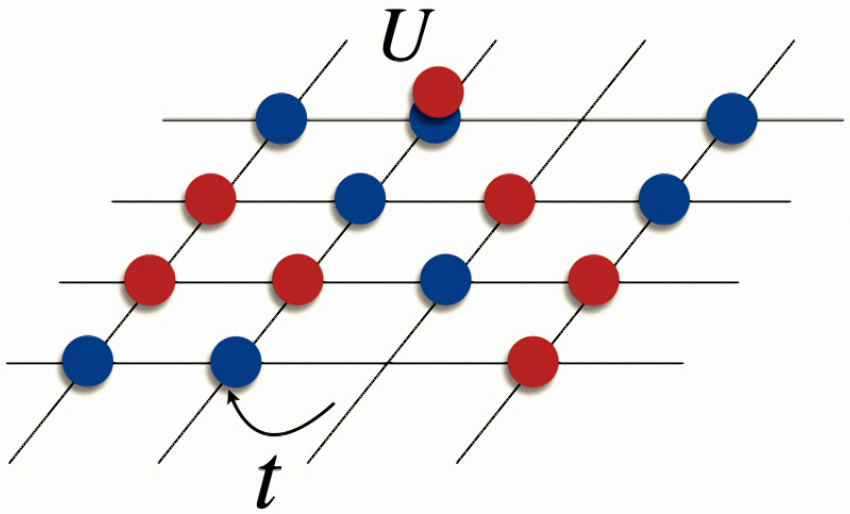
Quantum many-body systems



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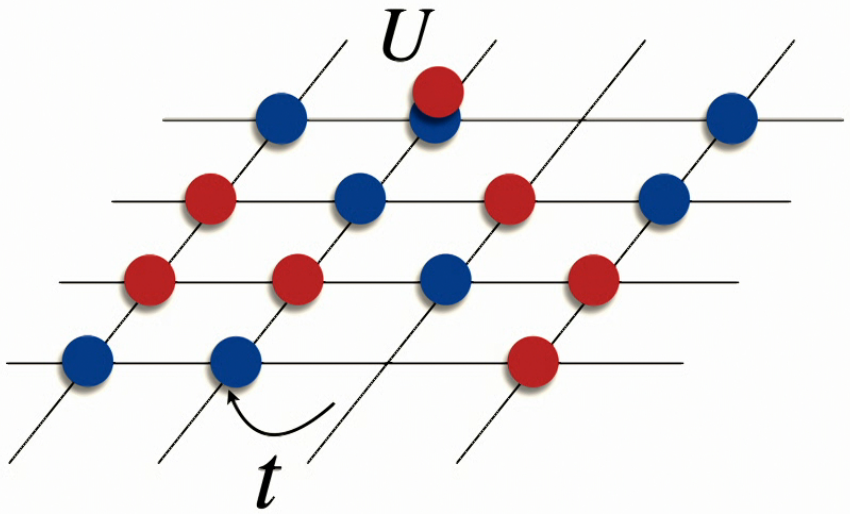
Quantum many-body systems



$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + h.c. \right) + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

tunneling

interaction

Simple set of rules:

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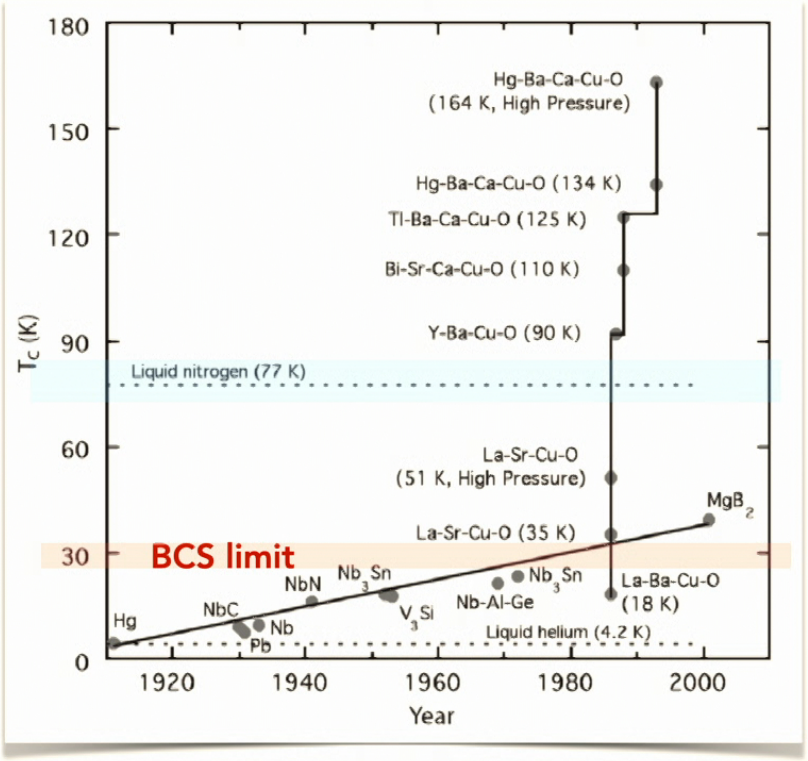
Why should you care

High-temperature superconductivity:



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Why should you care

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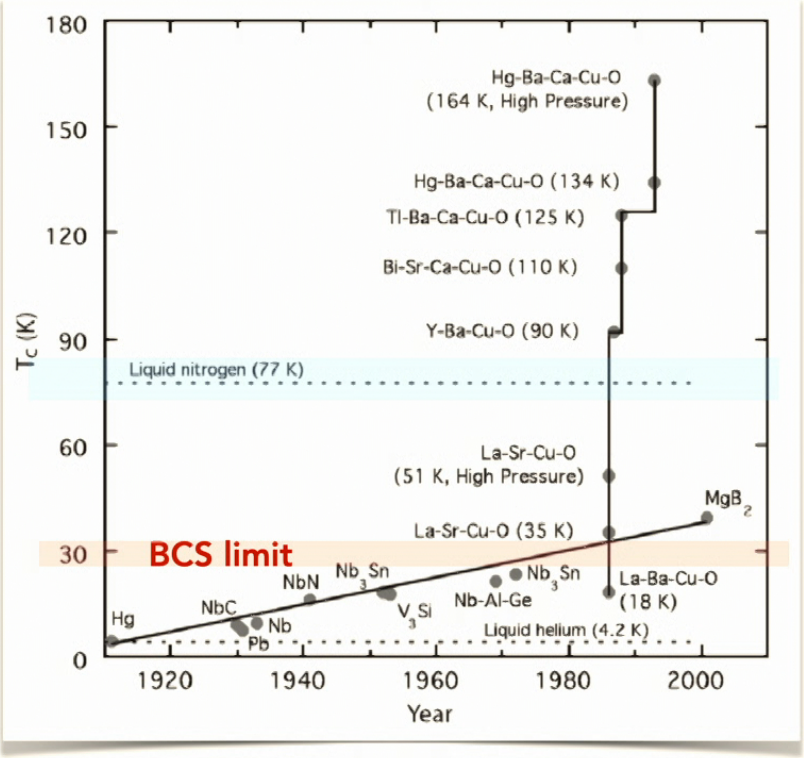
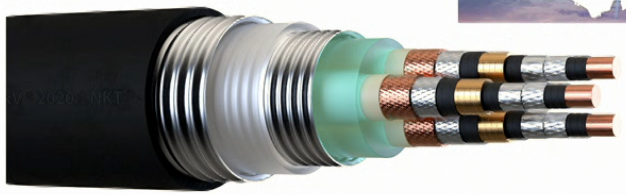


* ***Latest applications:***

Munich's SuperLink
SC cable (12 km)



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Why should you care

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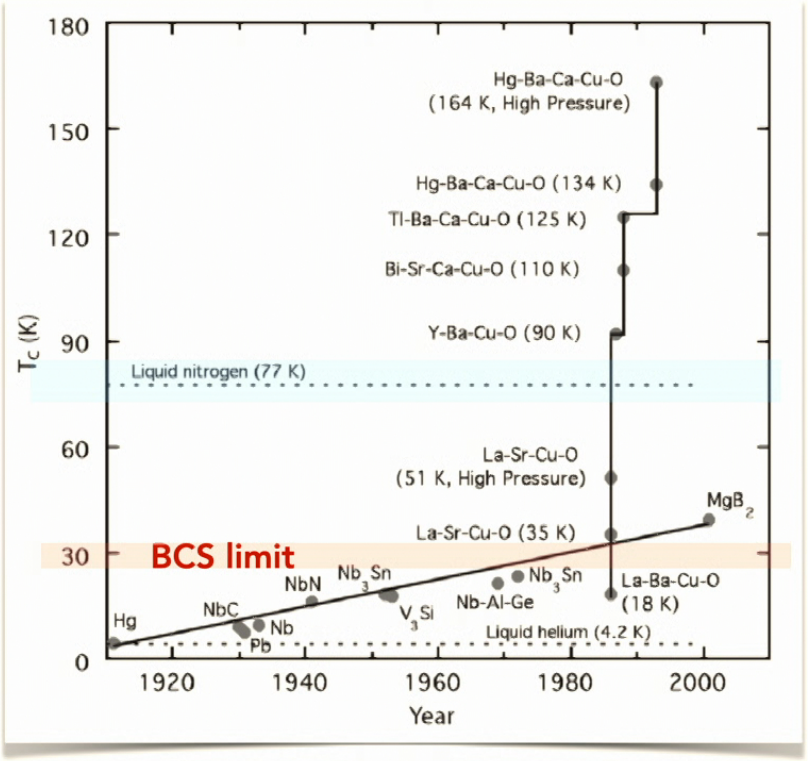

* ***Latest applications:***

Munich's SuperLink
SC cable (12 km)

* ***High-Tc wind turbine!***

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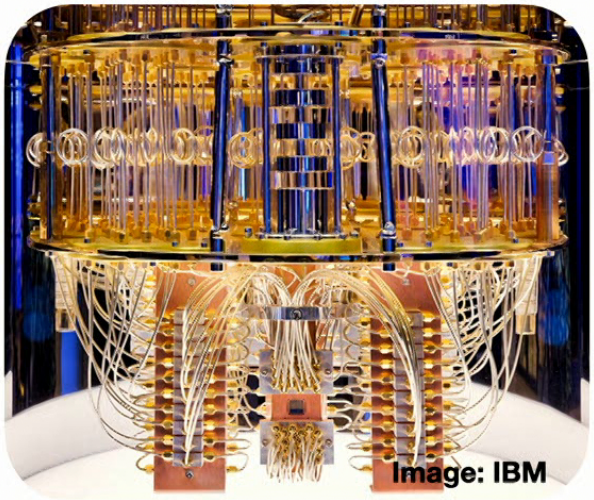
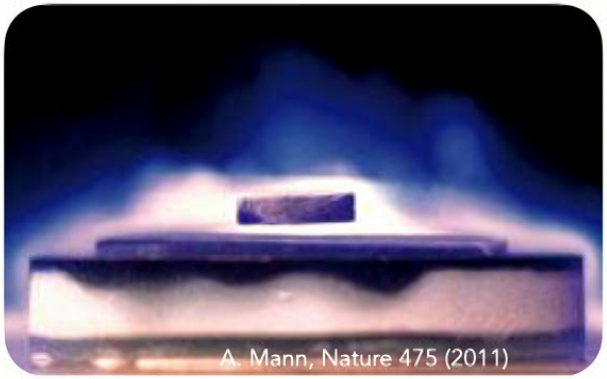
Why should you care

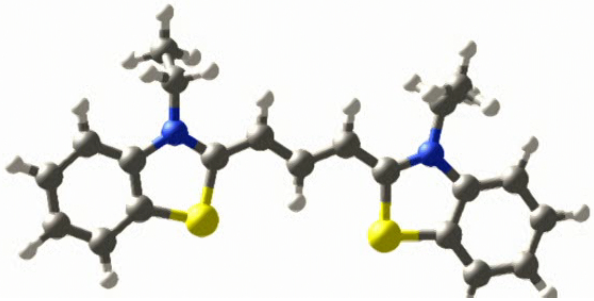
Quantum computing



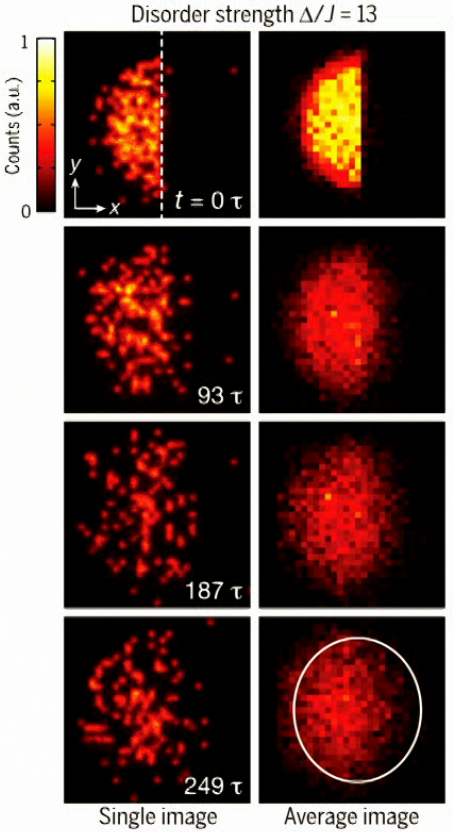
Materials research



Quantum chemistry

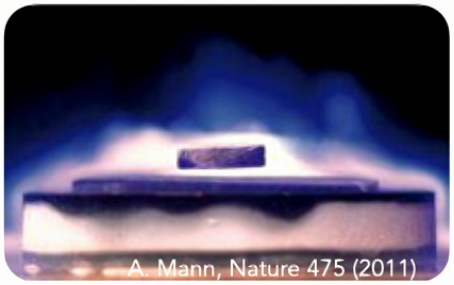


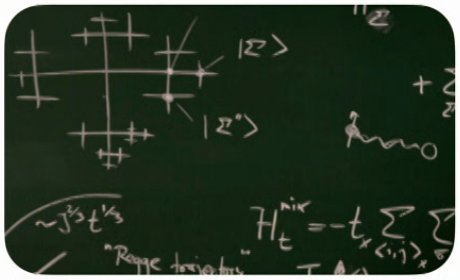
Fundamental research

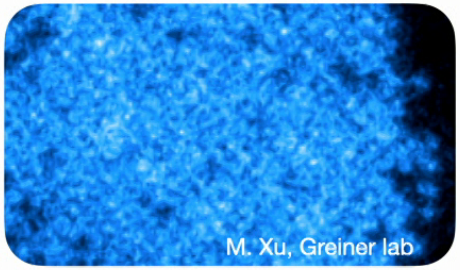


Choi et al., Science (2016)

What can we do?







Experiments on real materials (messy)

Analytical approximations

Numerical simulations

- Exact for small systems
- Approximations for large systems: what to throw away?

Quantum simulation

- What should we look for?

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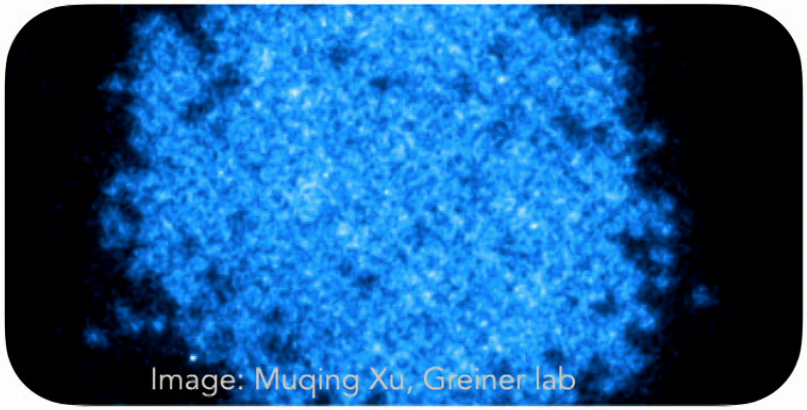
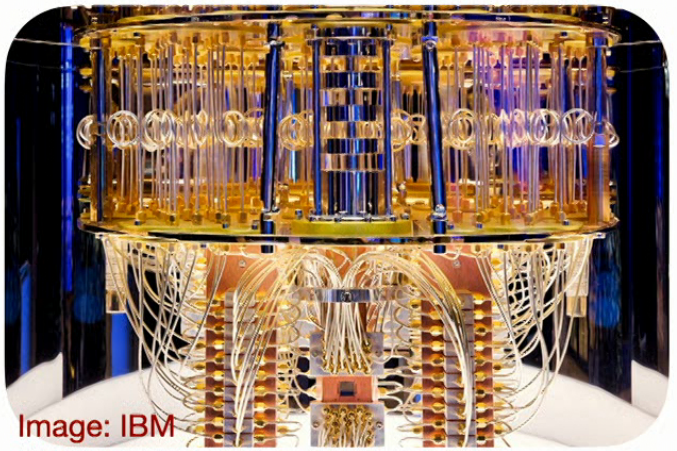
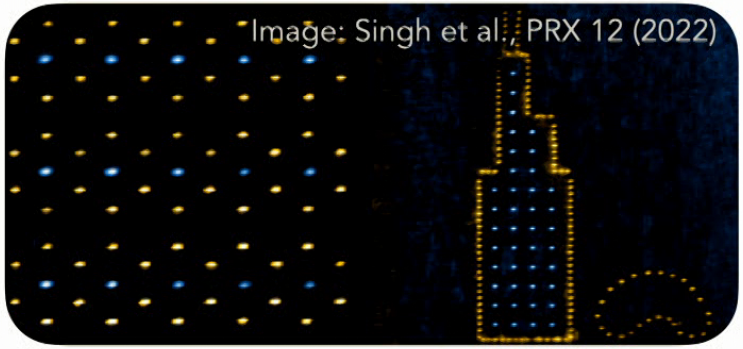
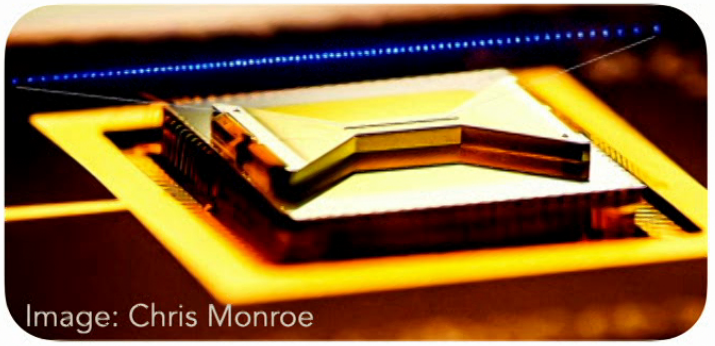
Quantum simulation









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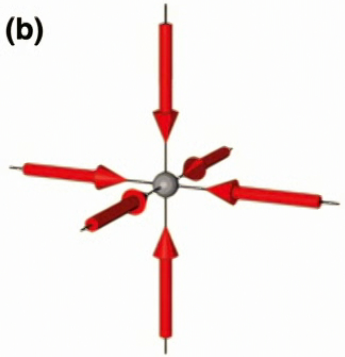
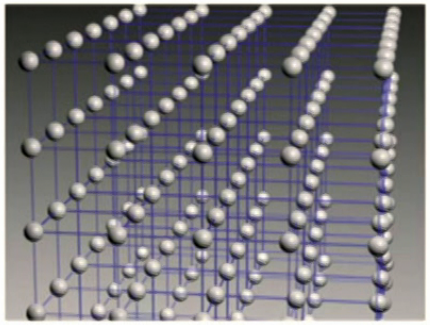
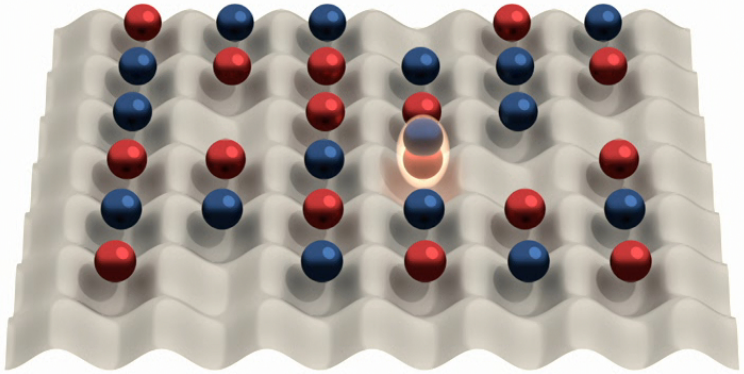
Cold atoms in optical lattices

Solid crystal: describe electrons moving in a periodic potential created by ions

Neutral atoms in a periodic potential created by interfering laser beams







Early review: Bloch & Zwerger, Rev Mod Phys. 80 (2008)
More recent review: Gross & Bloch, Science 357 (2017)

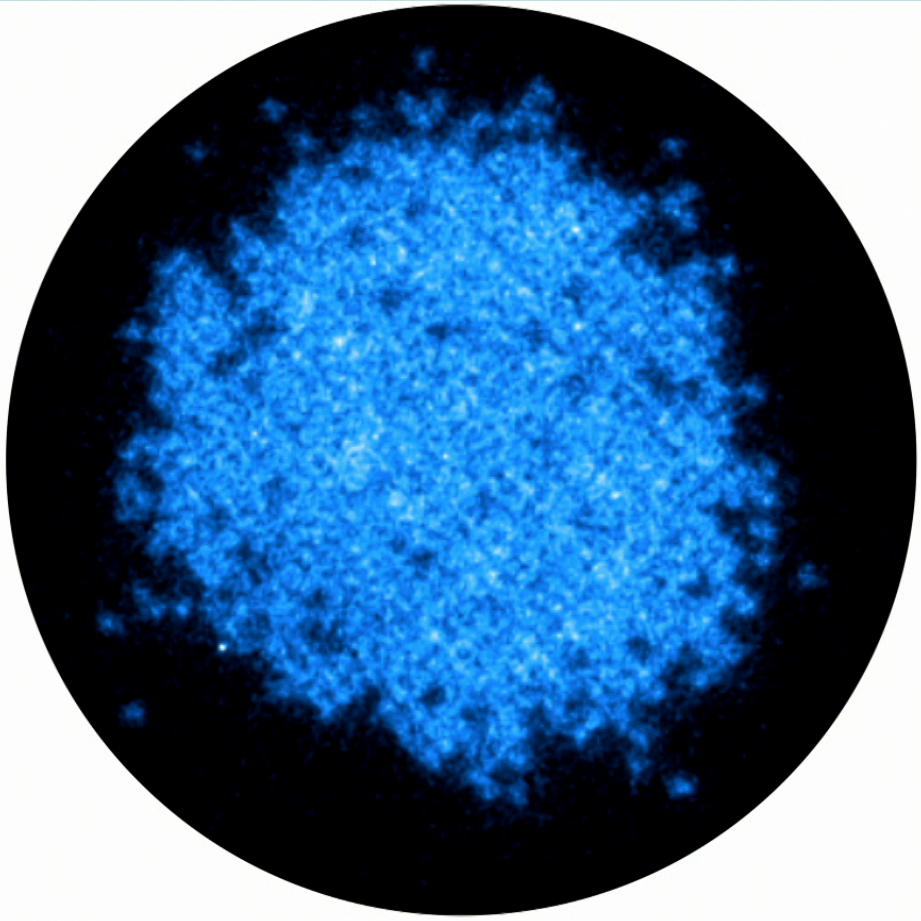


Image: Muqing Xu, Greiner lab

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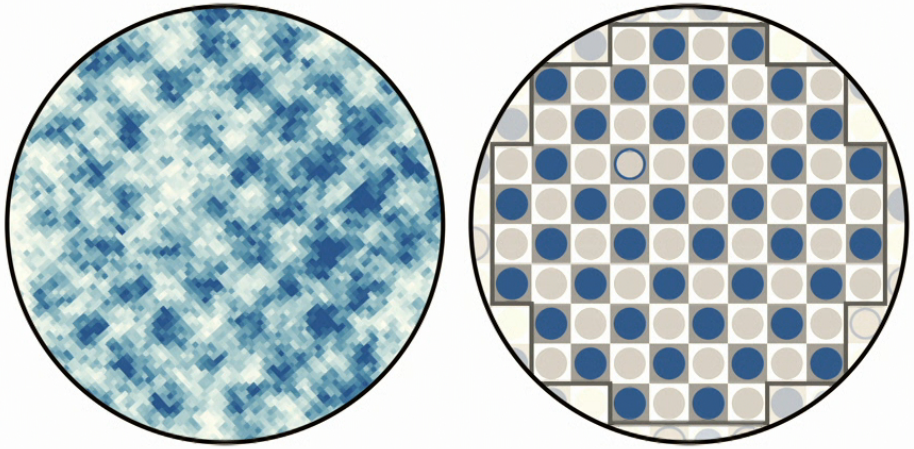
Quantum projective measurements

$$|\psi\rangle = |\;\;\rangle + |\;\;\rangle + |\;\;\rangle + |\;\;\rangle + \ldots$$



Mazurenko et al., Nature 545 (2017)

Outline

Getting a feeling for the Fermi-Hubbard model

A single hole — with a string attached

One, two, many holes?

(Interpretable) machine learning quantum snapshots

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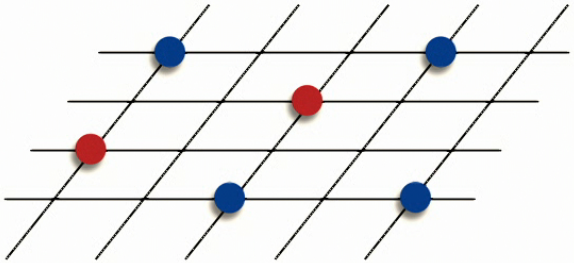
Fermi-Hubbard model

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + h.c. \right) + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

tunneling

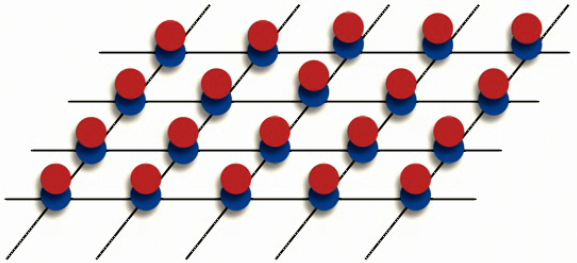
interaction

High temperatures:



metal

Increasing particle number



Band insulator

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Fermi-Hubbard model

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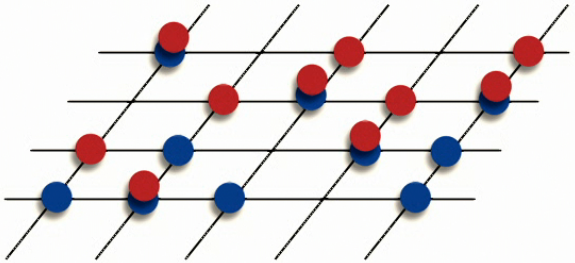
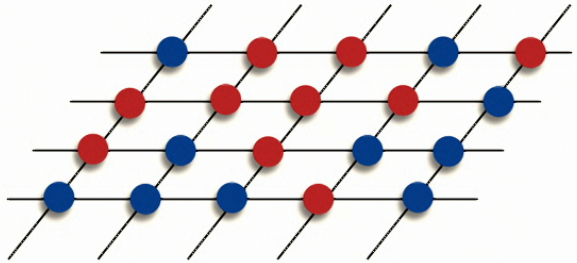
tunneling

interaction

Half-filling



Decreasing temperature $T < U$



metal

Mott insulator

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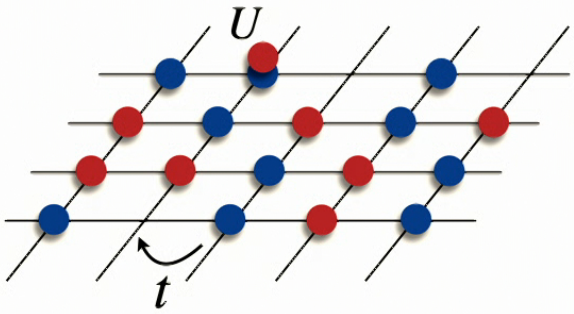
Fermi-Hubbard model



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tunneling — interaction

Large U limit: $t - J$ model

$$\hat{H}_{t-J} = -t \hat{P} \Big[\sum_{\langle \mathbf{i},\mathbf{j} \rangle, \sigma} \hat{c}^{\dagger}_{\mathbf{i},\sigma} \hat{c}_{\mathbf{j},\sigma} + \mathrm{h.c.} \Big] \hat{P} + J \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \left(\hat{\mathbf{S}}_{\mathbf{i}} \cdot \hat{\mathbf{S}}_{\mathbf{j}} - \frac{1}{4} \hat{n}_{\mathbf{i}} \hat{n}_{\mathbf{j}} \right)$$

no double-occupancies — tunneling — spin-exchange

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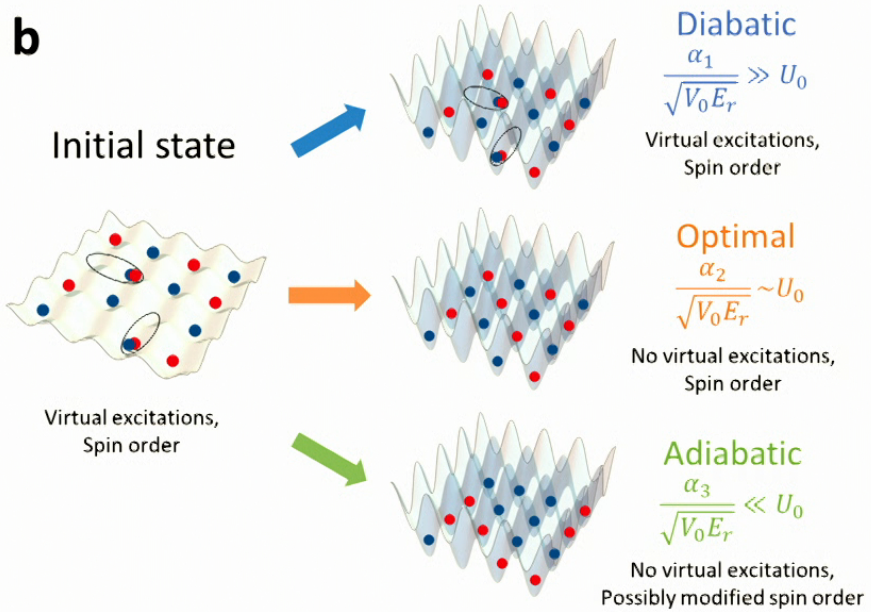
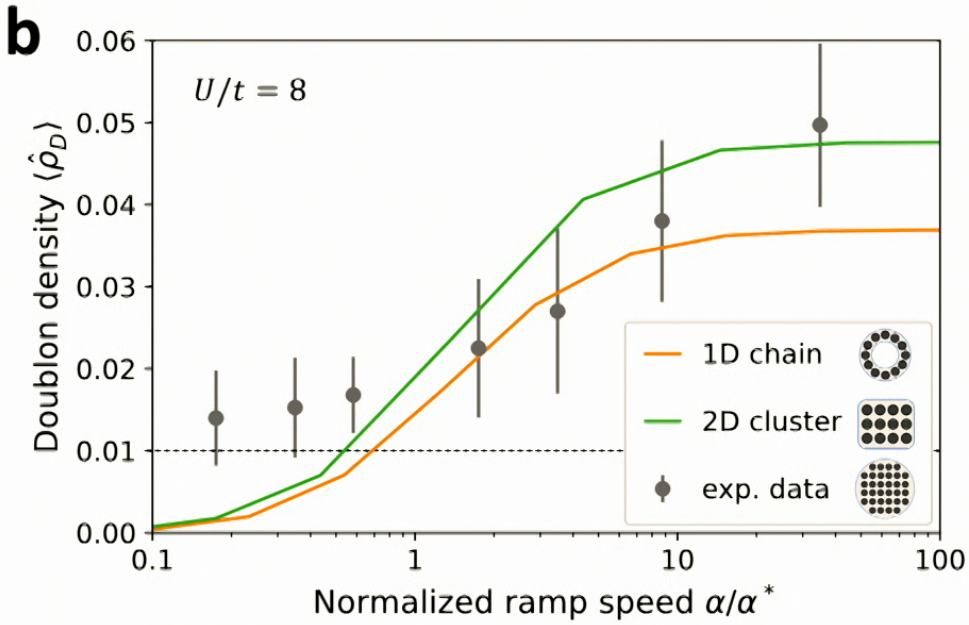
Experimental Schrieffer Wolff transformation





Kale et al., PRA 106 (2022)

see also: active learning for adaptive basis choices: Lange et al., arXiv:2203.15719

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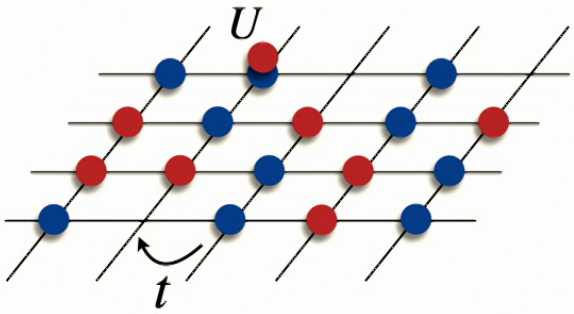
Fermi-Hubbard model



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tunneling — interaction

temperature

Large U limit: $t - J$ model

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no double-occupancies — tunneling — spin-exchange

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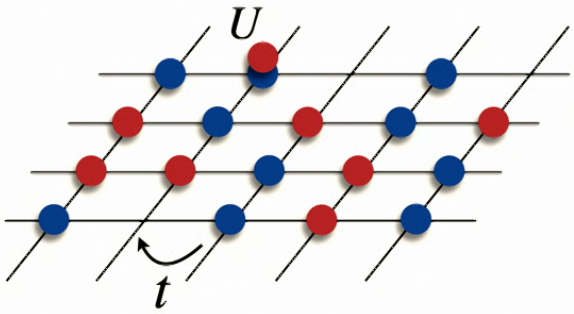
Fermi-Hubbard model



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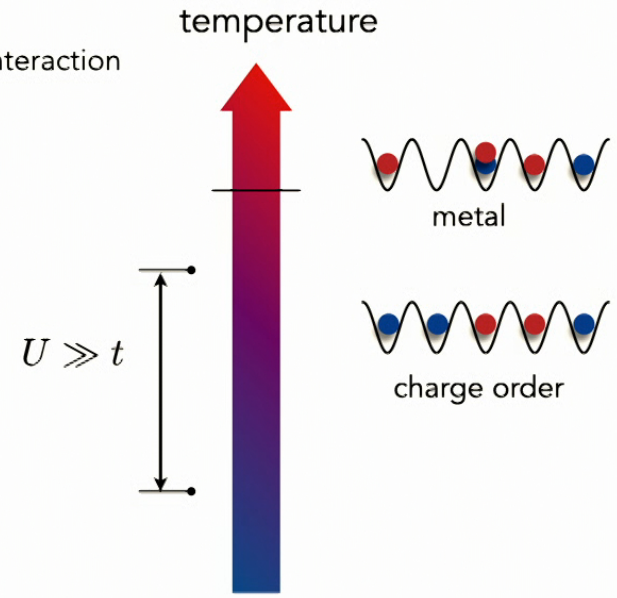
no double-occupancies — tunneling — spin-exchange



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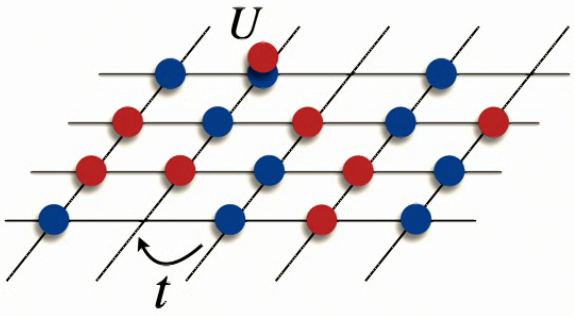
Fermi-Hubbard model



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tunneling — interaction

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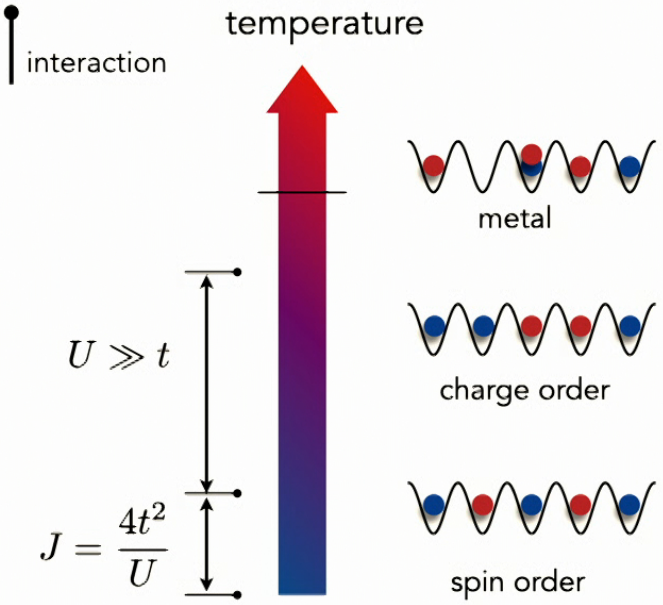
no double-occupancies — tunneling — spin-exchange



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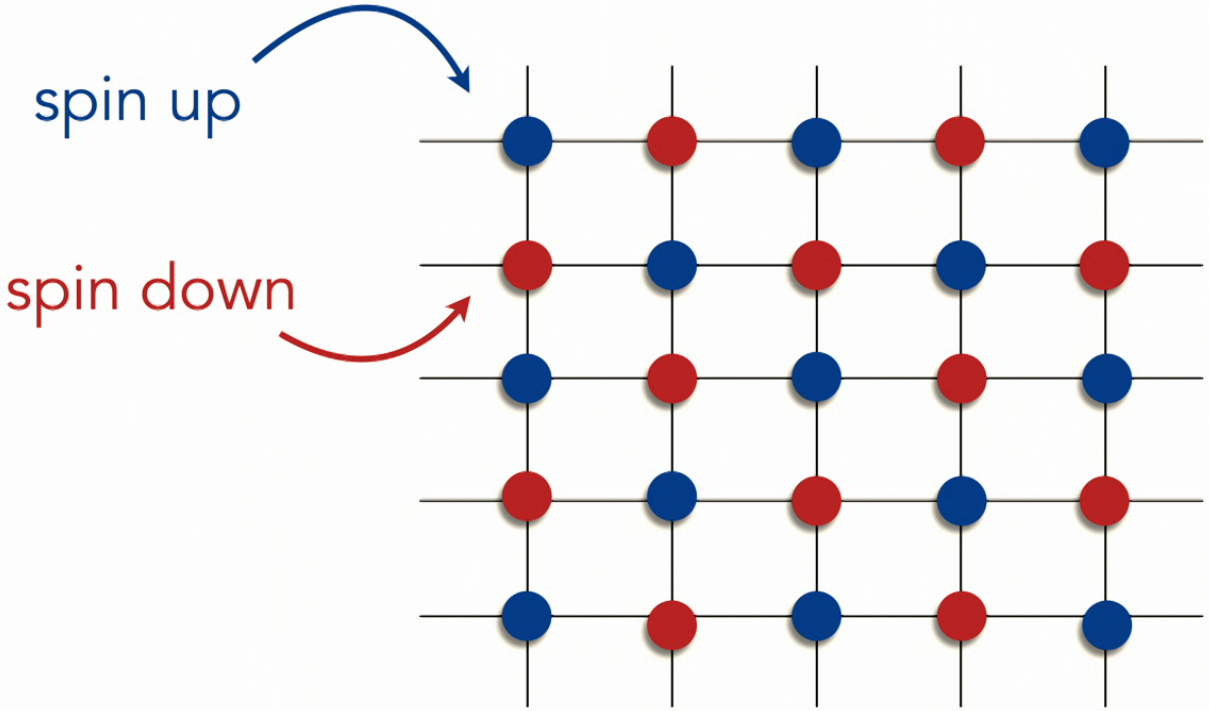
Antiferromagnetism



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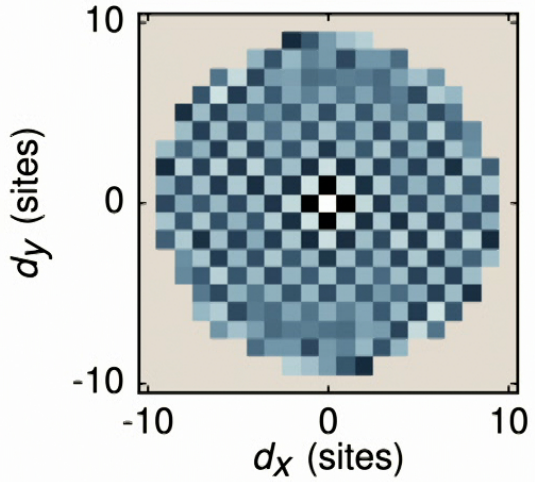
Fermi-Hubbard model

Antiferromagnet

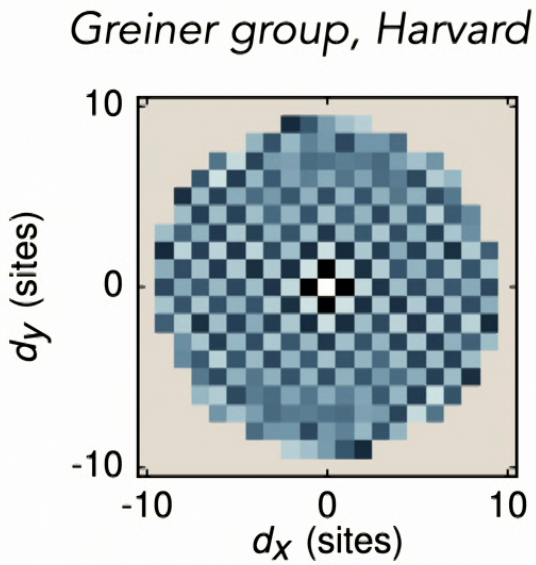
Greiner group, Harvard



Mazurenko et al., Nature 545 (2017)

Fermi-Hubbard model

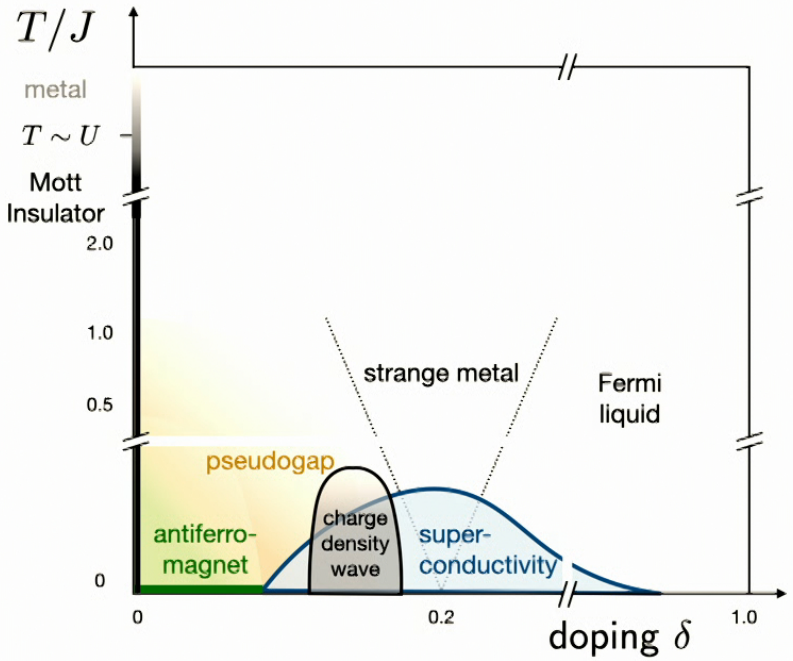
Antiferromagnet

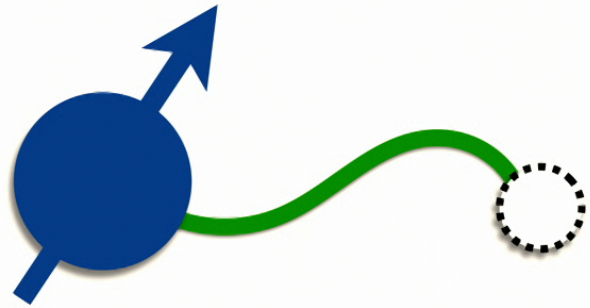


Mazurenko et al., Nature 545 (2017)

Review article: Fermi-Hubbard with cold atoms

Bohrdt et al., Annals of Physics (2021)





A single hole

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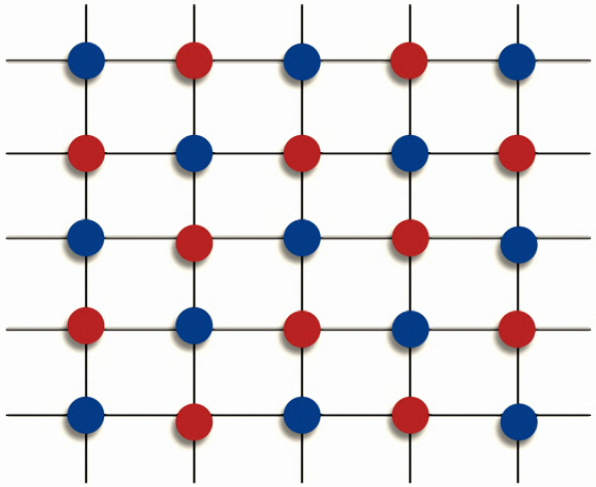
Geometric string theory



Grusdt et al., PRX 8 (2018), Grusdt et al., PRB 99 (2019), Bohrdt et al., NJP 22 (2020)

Early work: Bulaevskii et al., JETP 27 (1968), Trugman, PRB 37 (1988), Manousakis, PRB 75 (2007)

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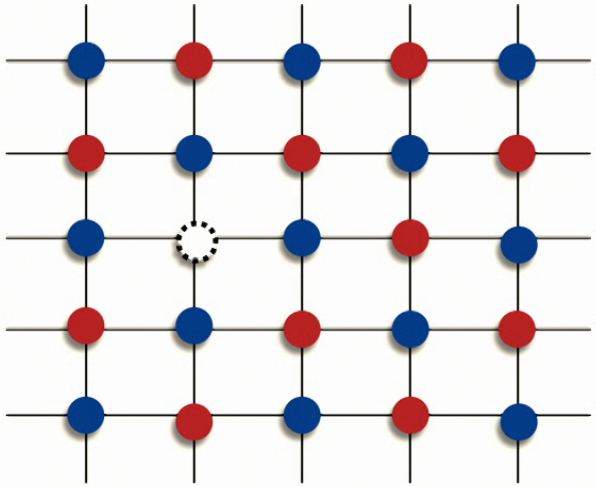
Geometric string theory



Grusdt et al., PRX 8 (2018), Grusdt et al., PRB 99 (2019), Bohrdt et al., NJP 22 (2020)

Early work: Bulaevskii et al., JETP 27 (1968), Trugman, PRB 37 (1988), Manousakis, PRB 75 (2007)

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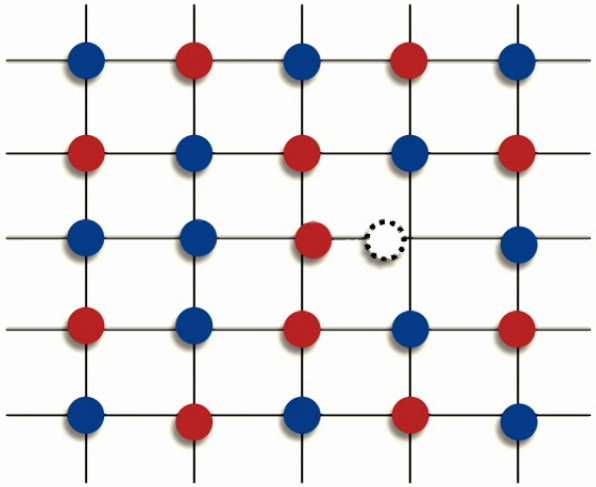
Geometric string theory



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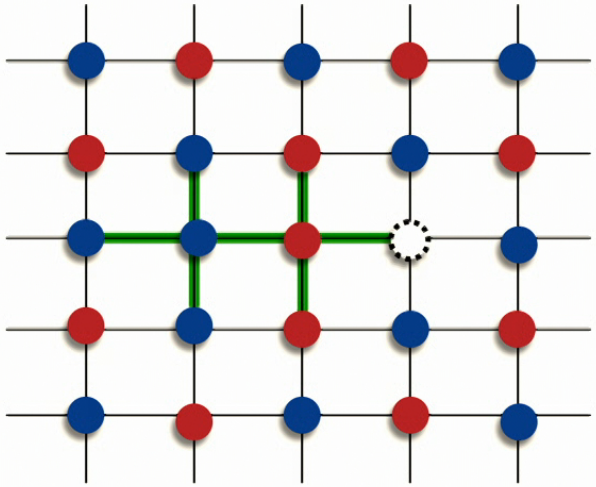

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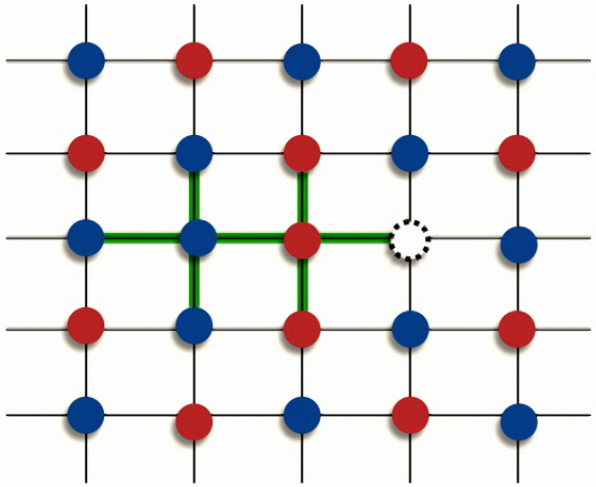

$$\frac{dE}{dl} = 2J\left(C_{\mathbf{e}_x+\mathbf{e}_y} - C_{\mathbf{e}_x}\right)$$

Grusdt et al., PRX 8 (2018), Grusdt et al., PRB 99 (2019), Bohrdt et al., NJP 22 (2020)

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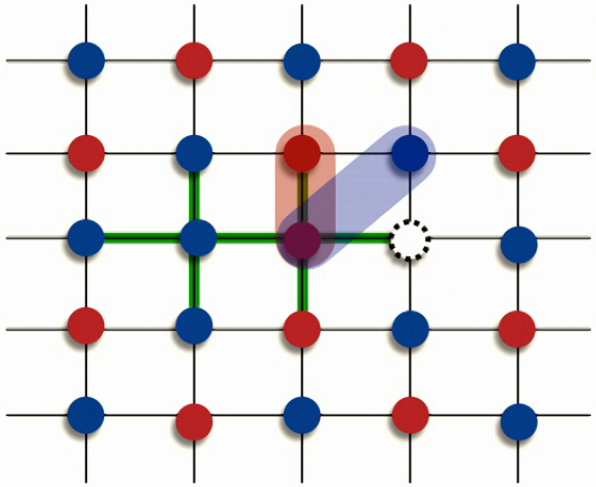

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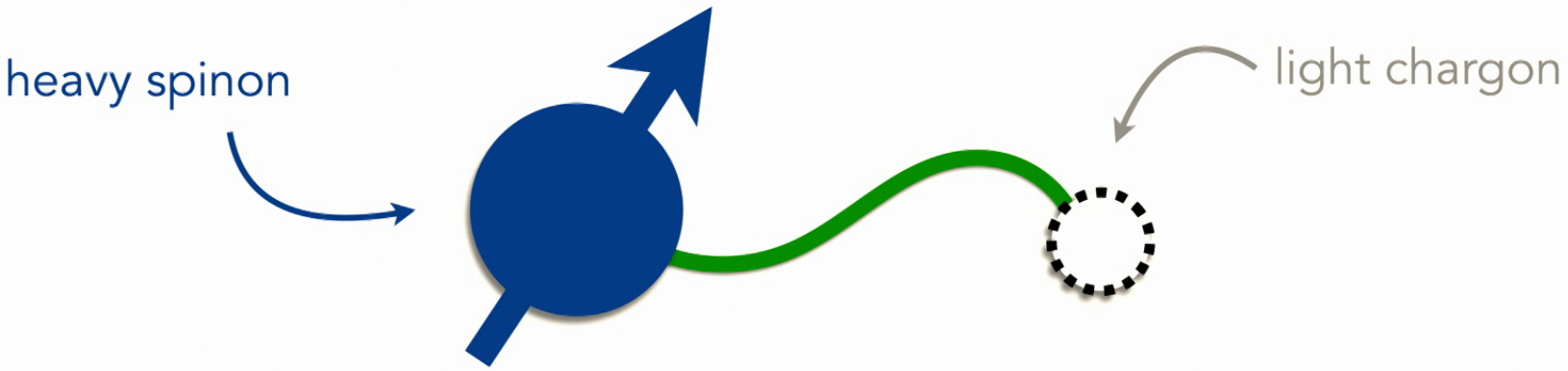
Geometric string theory

- Born-Oppenheimer approximation: $|\psi\rangle \simeq |\psi_{\text{spinon}}\rangle \otimes |\psi_{\text{string}}\rangle$



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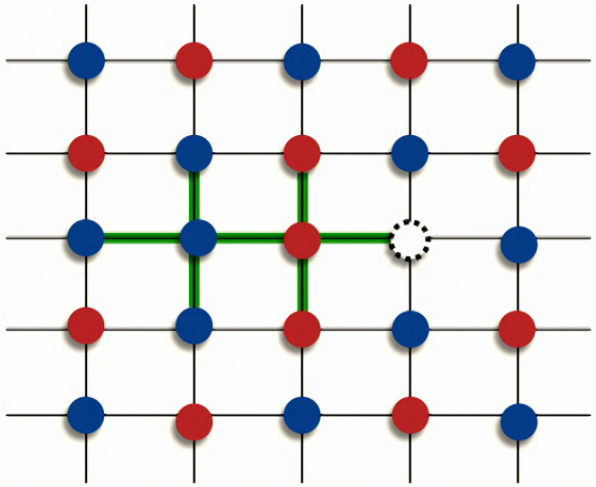
Geometric string theory



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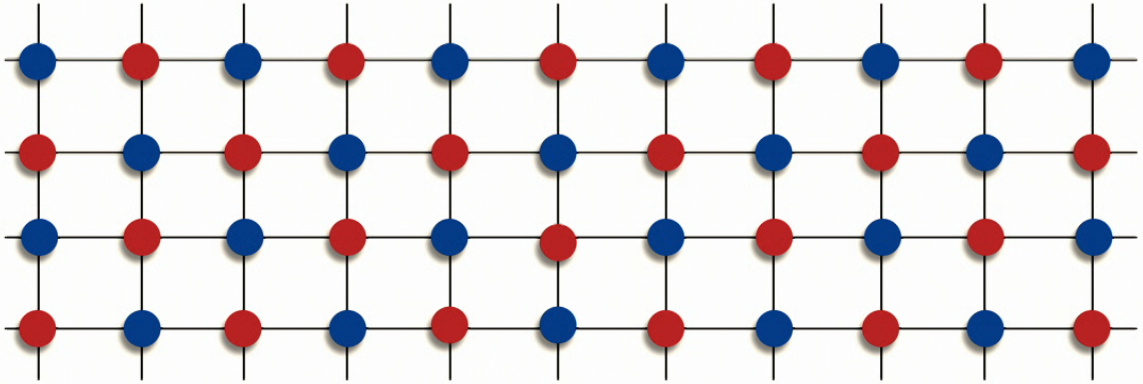

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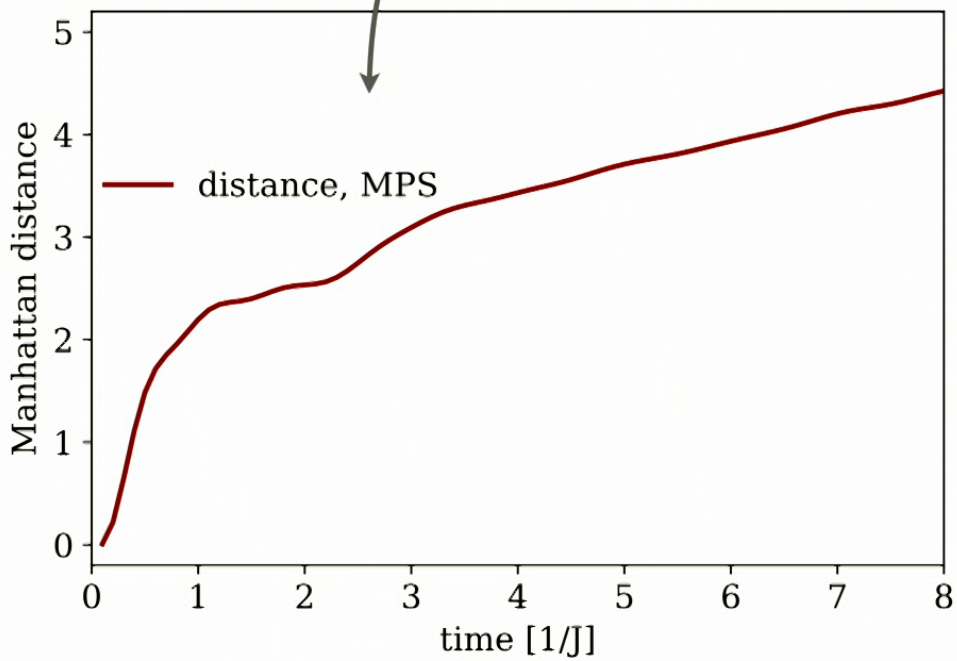
Hole dynamics

time-dependent **M**atrix **P**roduct **S**tate simulations of the microscopic Hamiltonian



Bohrdt et al., NJP 22 (2020)

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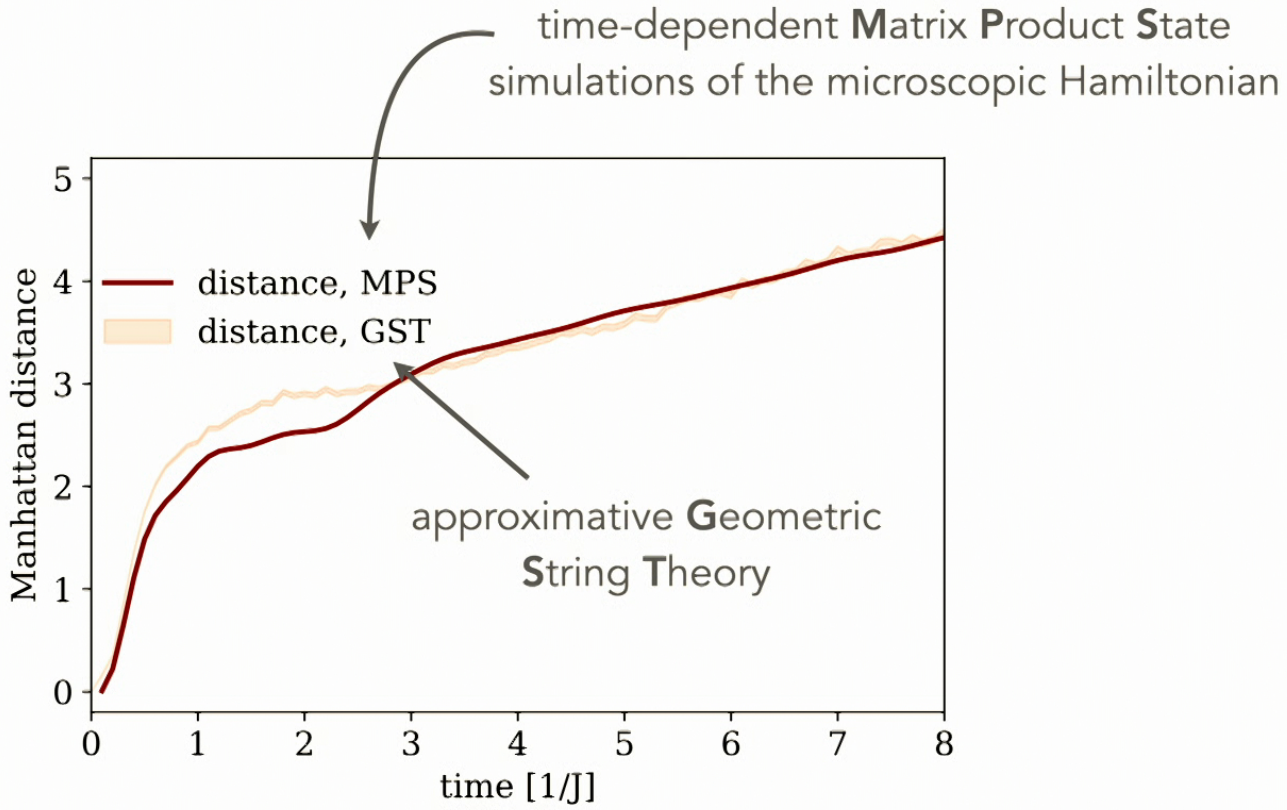
Hole dynamics



Bohrdt et al., NJP 22 (2020)

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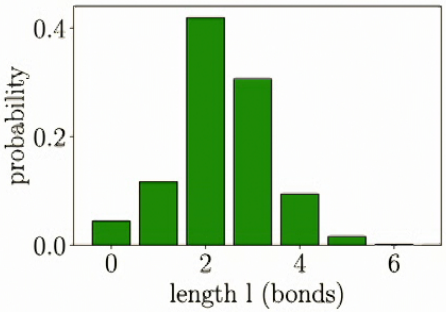
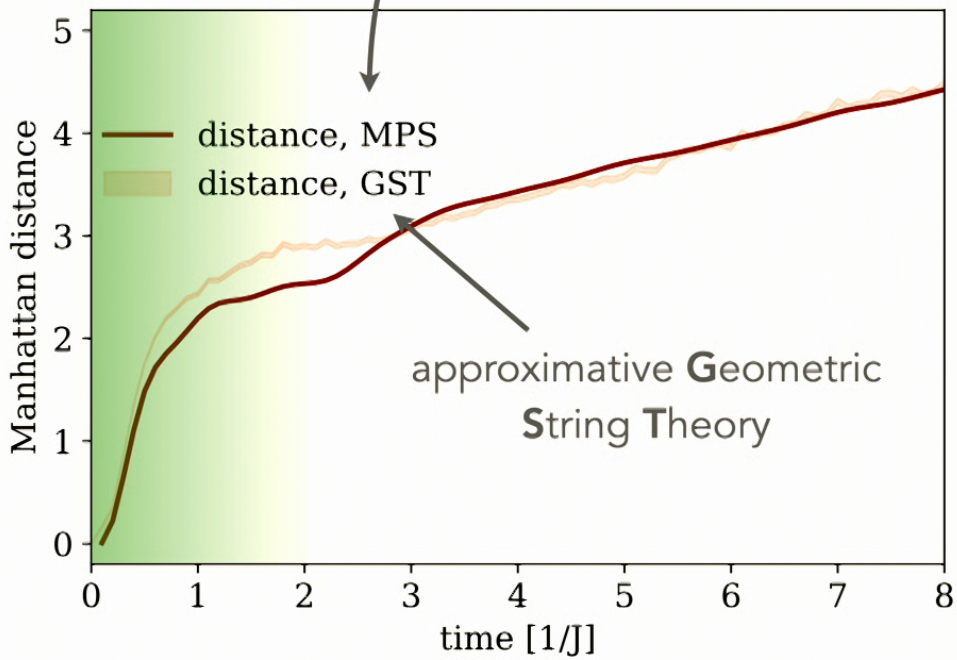
Hole dynamics

String formation



time-dependent **M**atrix **P**roduct **S**tate simulations of the microscopic Hamiltonian



Bohrdt et al., NJP 22 (2020)

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Hole dynamics

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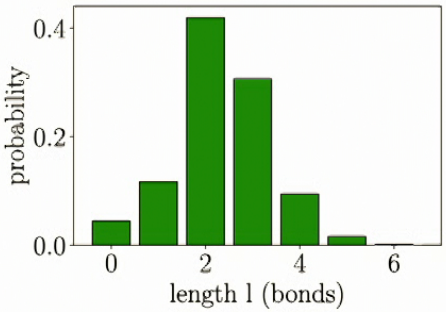
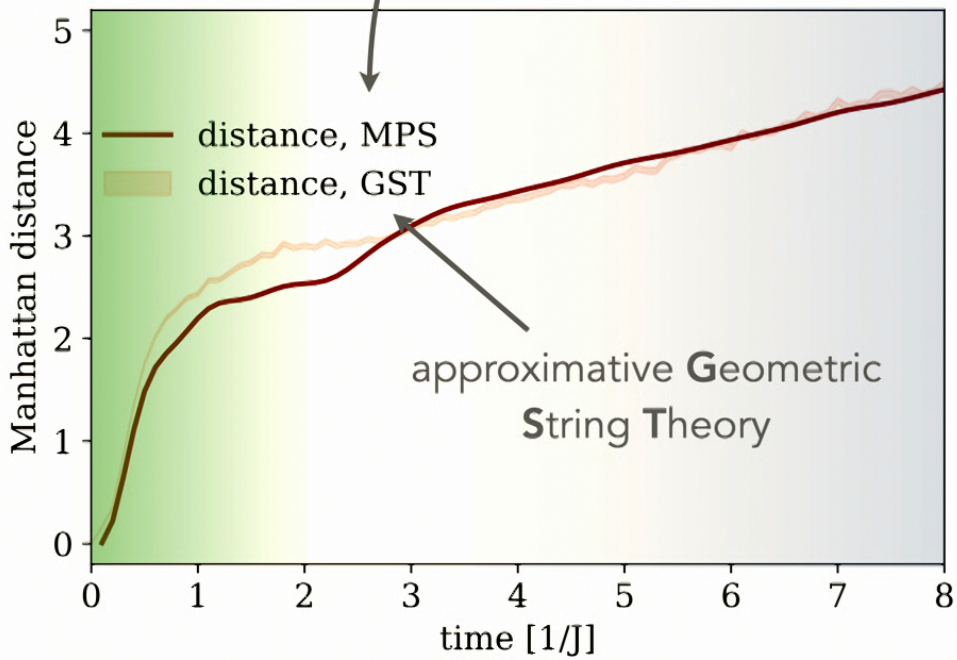


time-dependent **M**atrix **P**roduct **S**tate simulations of the microscopic Hamiltonian



Spinon dynamics

$$\hat{H}_{\mathrm{sp}} = \sum_{\mathbf{k},\sigma} \omega_{\mathrm{sp}} \hat{s}^{\dagger}_{\mathbf{k},\sigma} \hat{s}_{\mathbf{k},\sigma}$$

Bohrdt et al., NJP 22 (2020)

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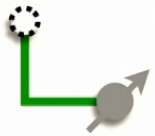
Quantum projective measurements

$$|\psi\rangle = |$$  $$\rangle + |$$  $$\rangle + |$$  $$\rangle + |$$  $$\rangle + \ldots$$

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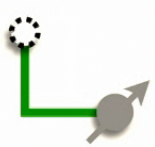
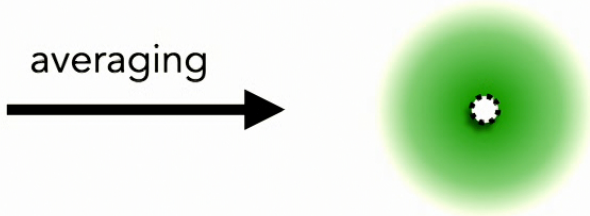
Quantum projective measurements

$|\psi\rangle = |$  $\rangle + |$  $\rangle + |$  $\rangle + |$  $\rangle + \ldots$

averaging



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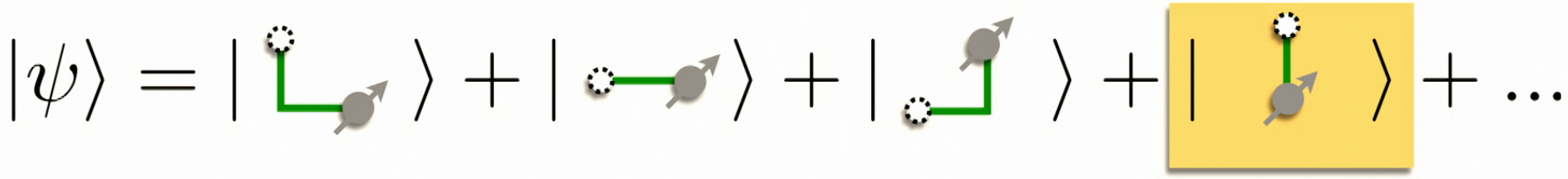
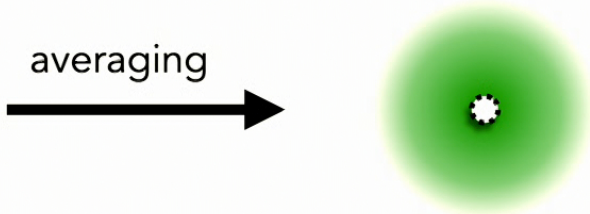
Quantum projective measurements





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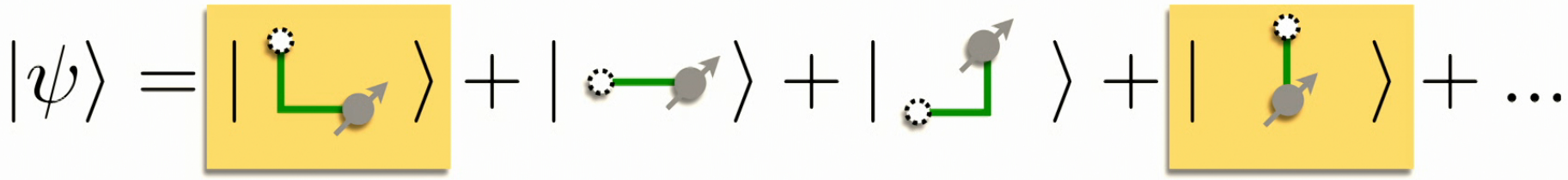
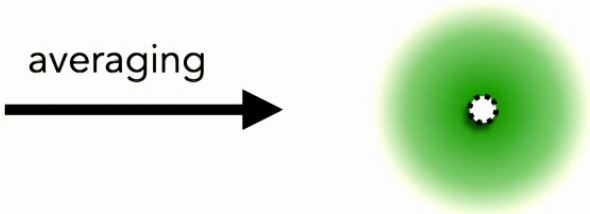
Quantum projective measurements



averaging



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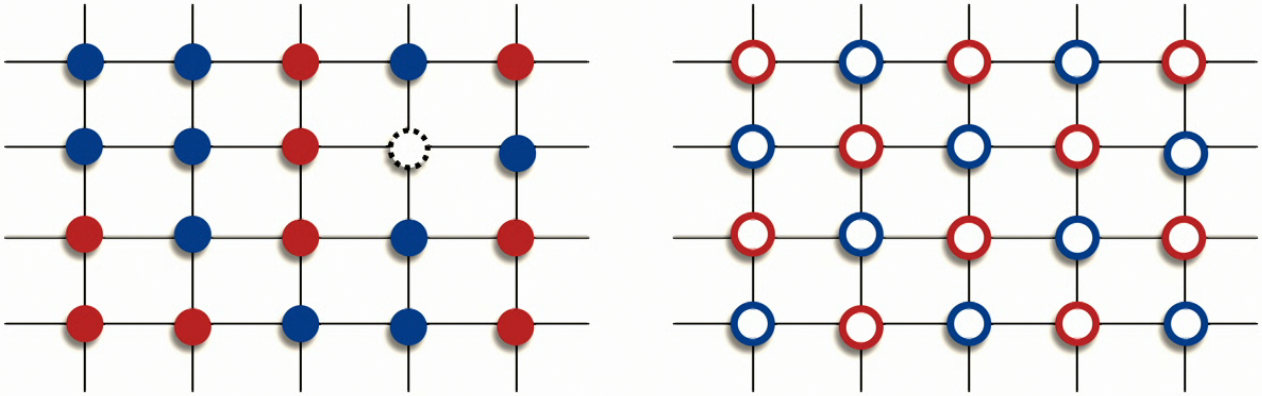
String patterns



Grusdt et al., PRX 8 (2018), Grusdt et al., PRB 99 (2019), Chiu et al., Science 365 (2019), Bohrdt et al., NJP 22 (2020)

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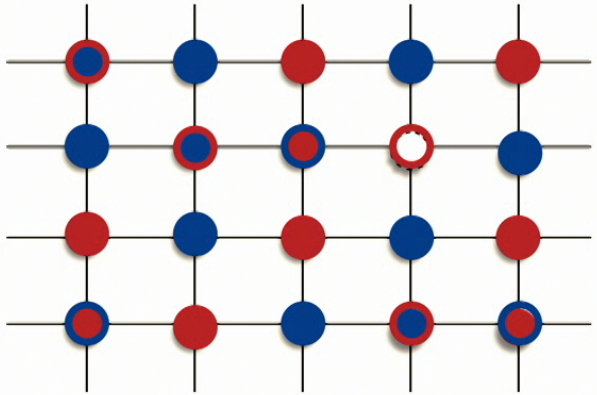

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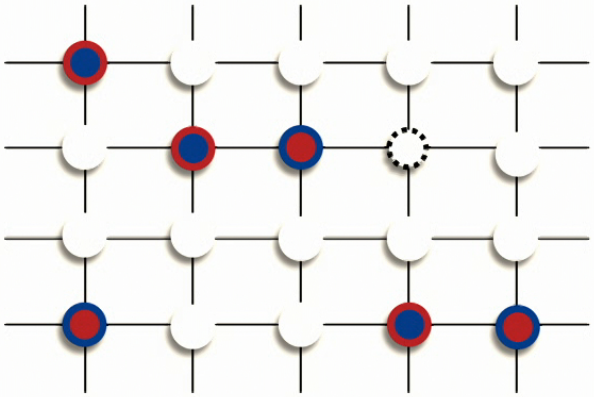

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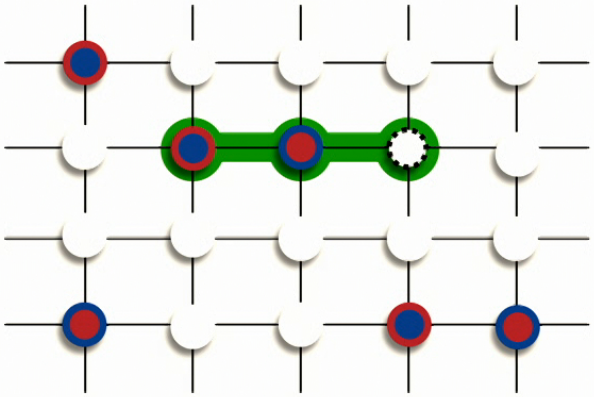

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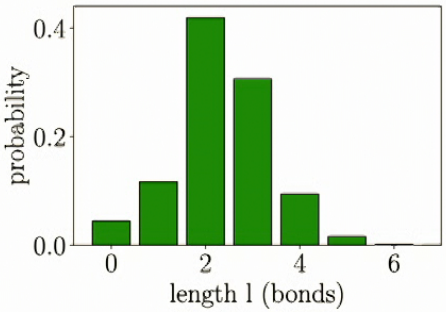
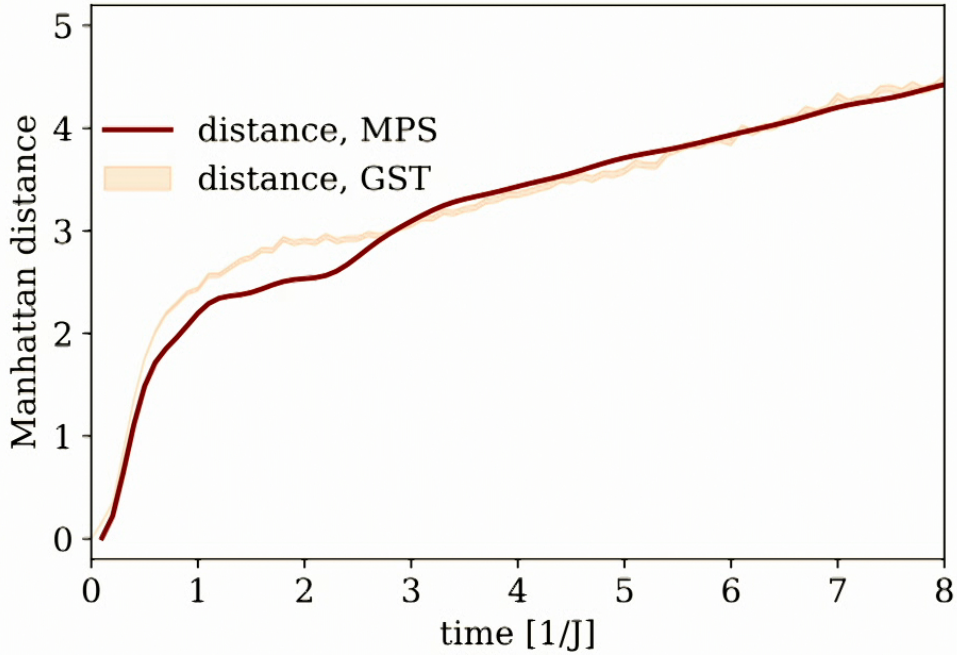
String patterns

String formation





Spinon dynamics

$$\hat{H}_{\mathrm{sp}} = \sum_{\mathbf{k},\sigma} \omega_{\mathrm{sp}} \hat{s}^{\dagger}_{\mathbf{k},\sigma} \hat{s}_{\mathbf{k},\sigma}$$

Bohrdt et al., NJP 22 (2020)

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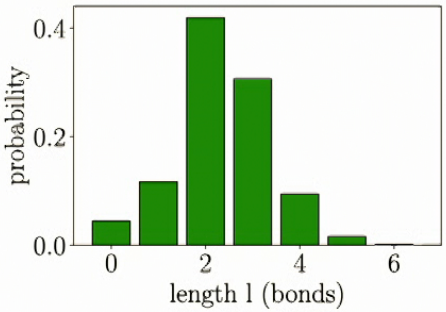

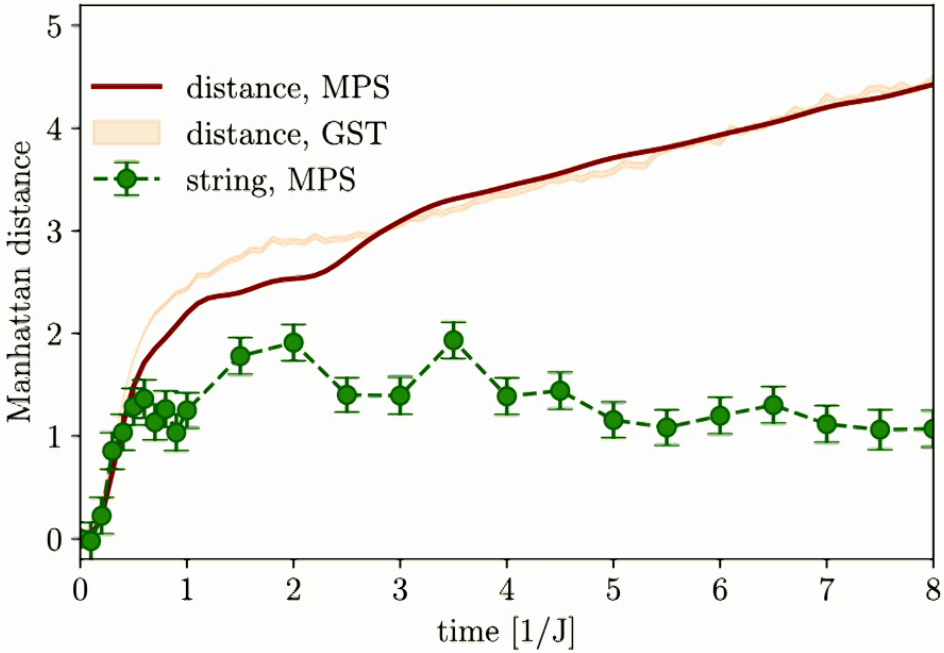

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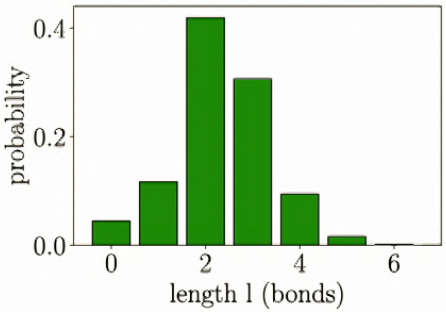

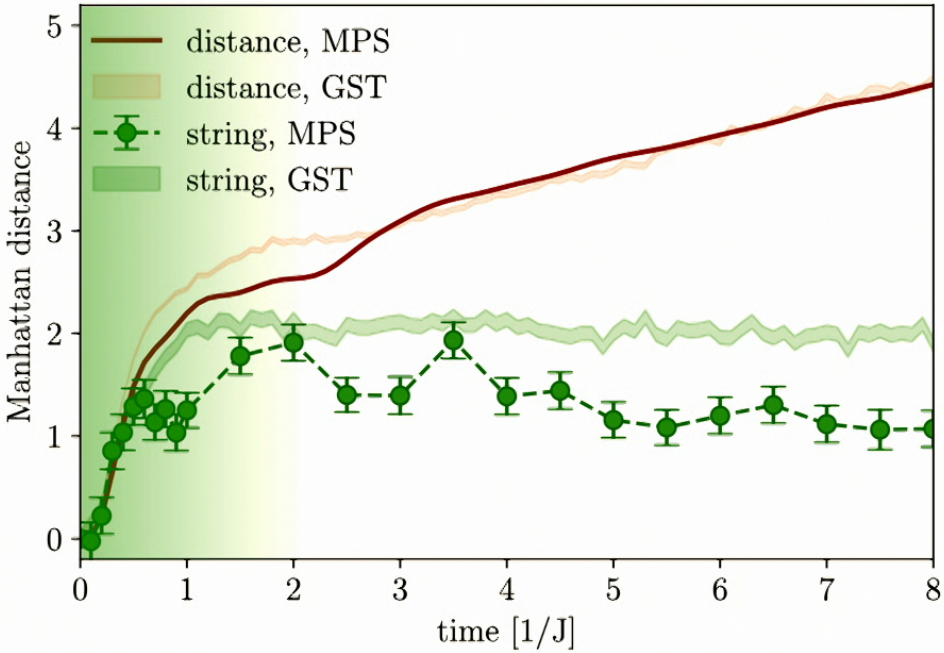

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Bohrdt et al., NJP 22 (2020)

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String patterns

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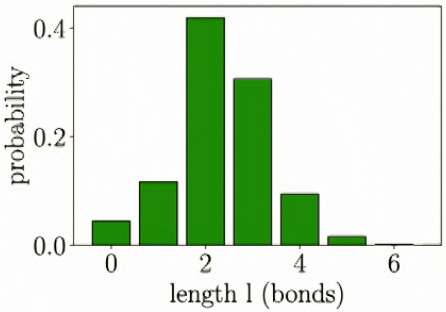

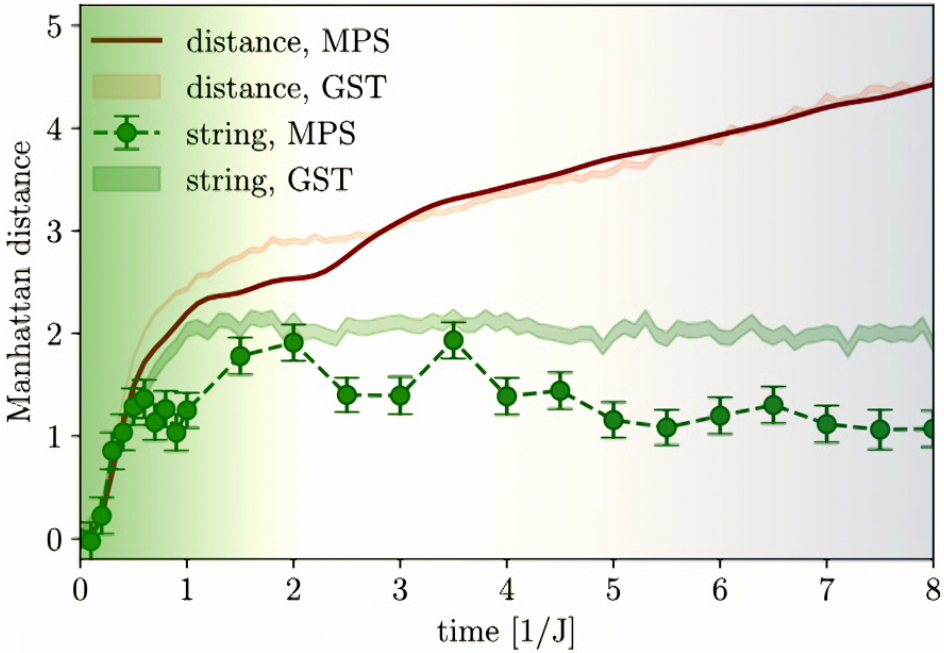

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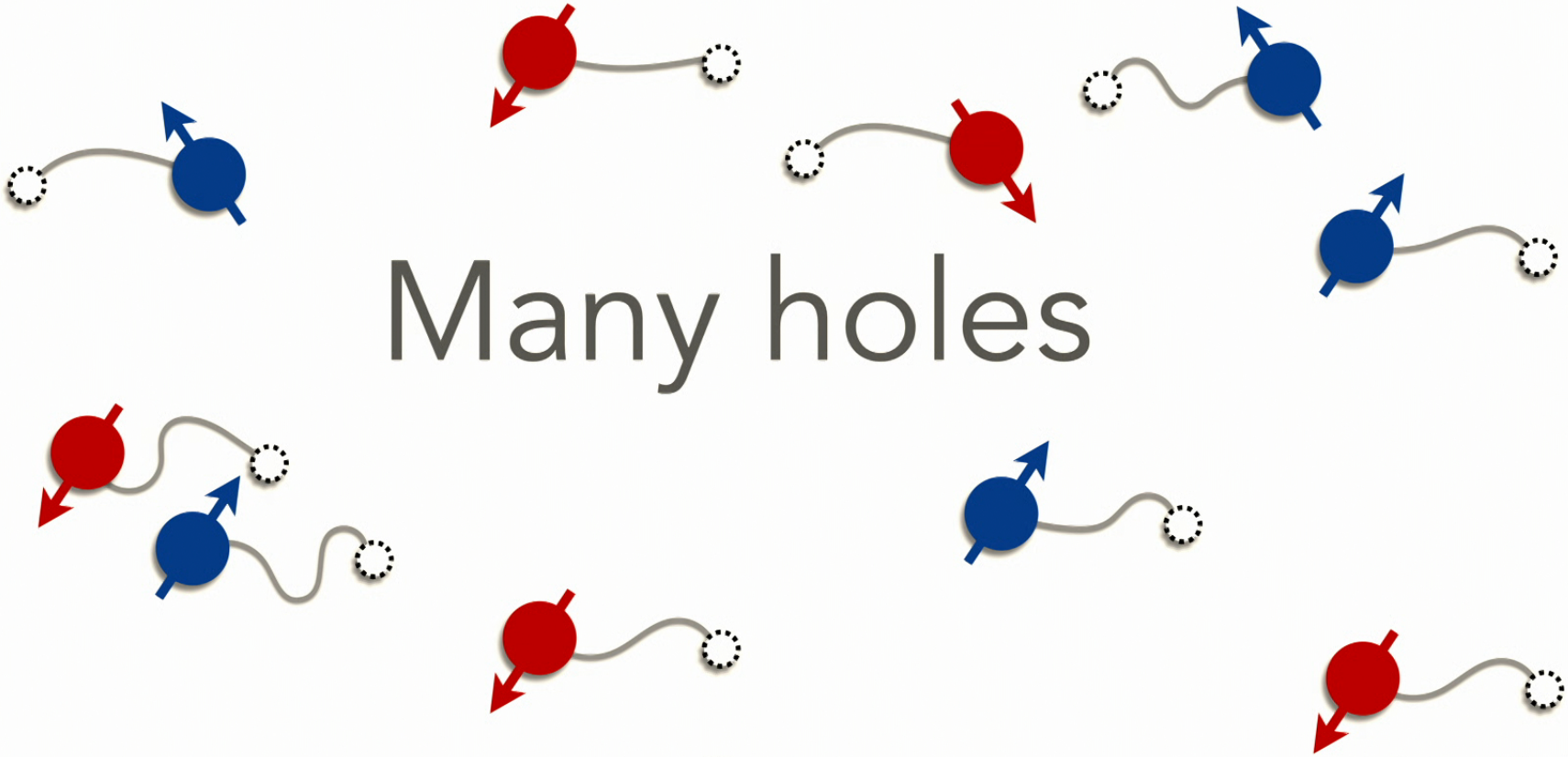
Bohrdt et al., NJP 22 (2020)



Many holes

Phase diagram

Numerics Review from last year:

2. Phase diagram and phase boundaries

Not much is known about the precise phase diagram of the Hubbard model in two dimensions. While the ground-state phase diagram of the model at weak coupling is fairly well understood (49, 266), the phase diagram in the intermediate-to-strong interaction limit is hotly debated. Determining precise phase boundaries is hindered by the fact that the diver-

Qin et al., Annual Review of Condensed Matter Physics 13 (2022)

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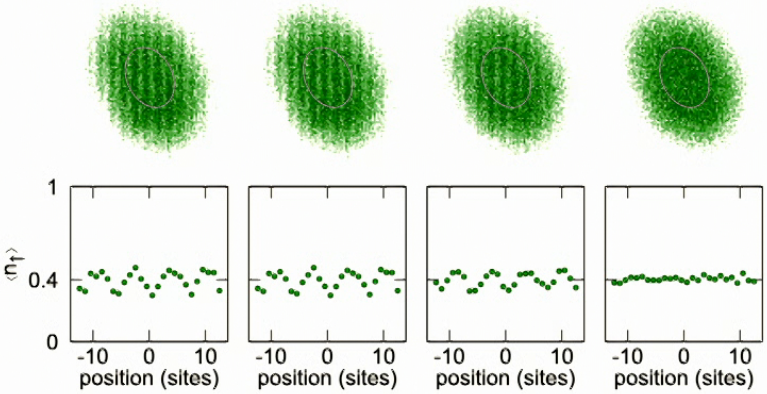
What should we look for?

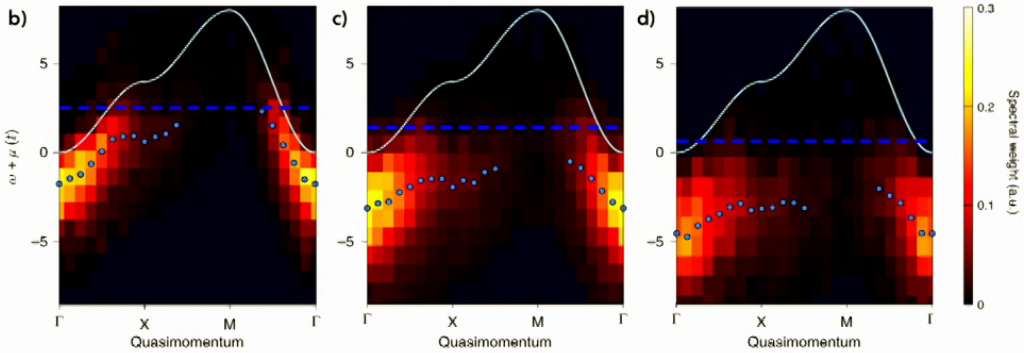
Option 1: Emulate solid state experiments

Transport properties



Brown et al., Science 363 (2019)

Angle resolved photoemission spectroscopy



Brown et al., Nature Physics 16 (2020)

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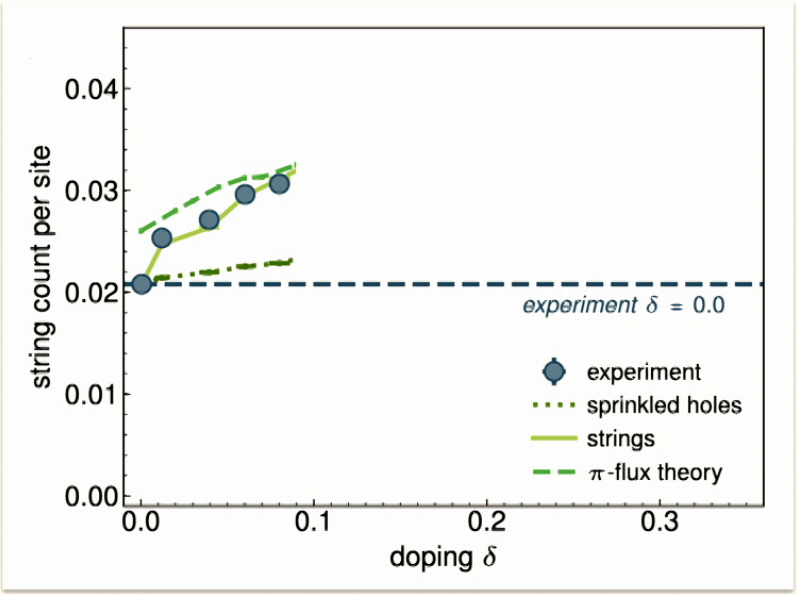
String patterns

Option 2: Make use of microscopic real-space information



C. Chiu et al., Science 365, 6450 (2019)

String patterns

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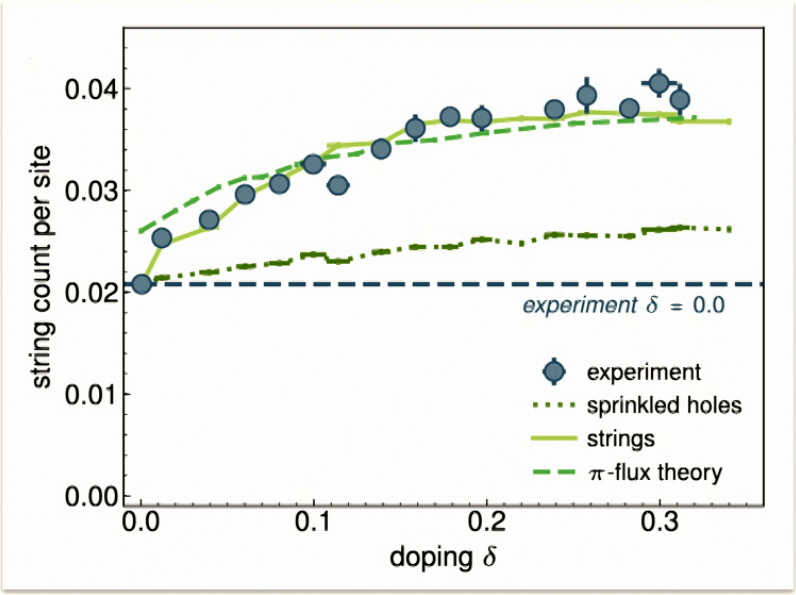

C. Chiu et al., Science 365, 6450 (2019)

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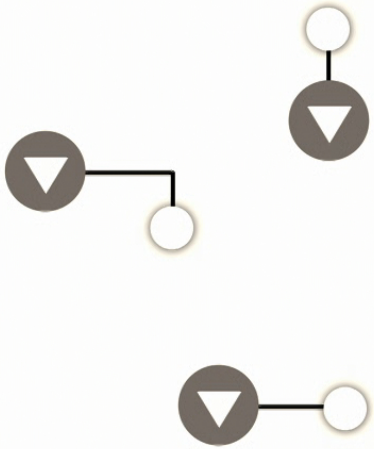

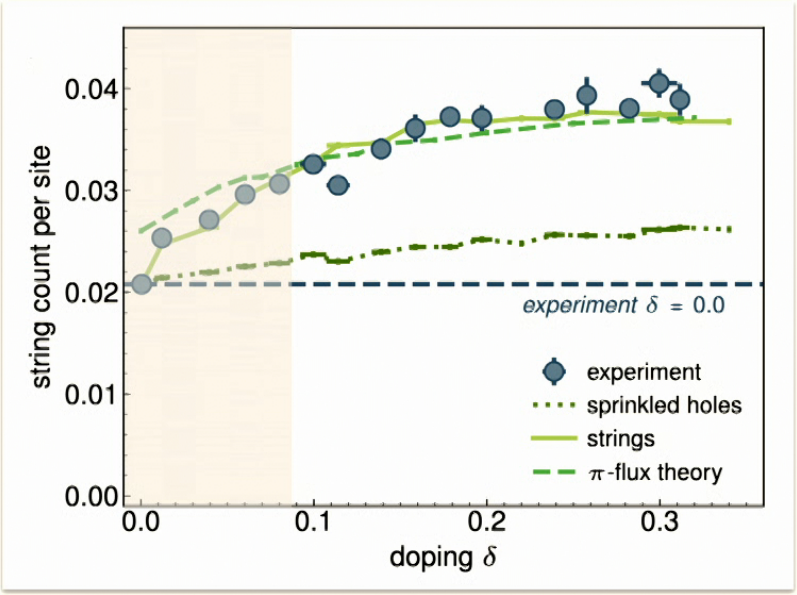

C. Chiu et al., Science 365, 6450 (2019)

String patterns

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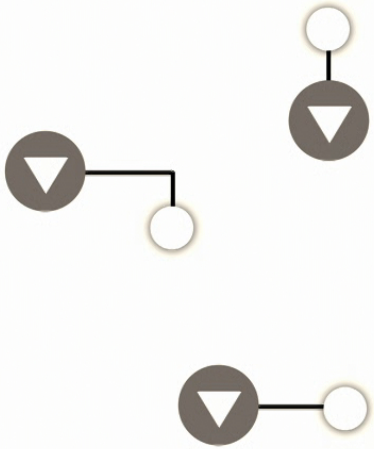

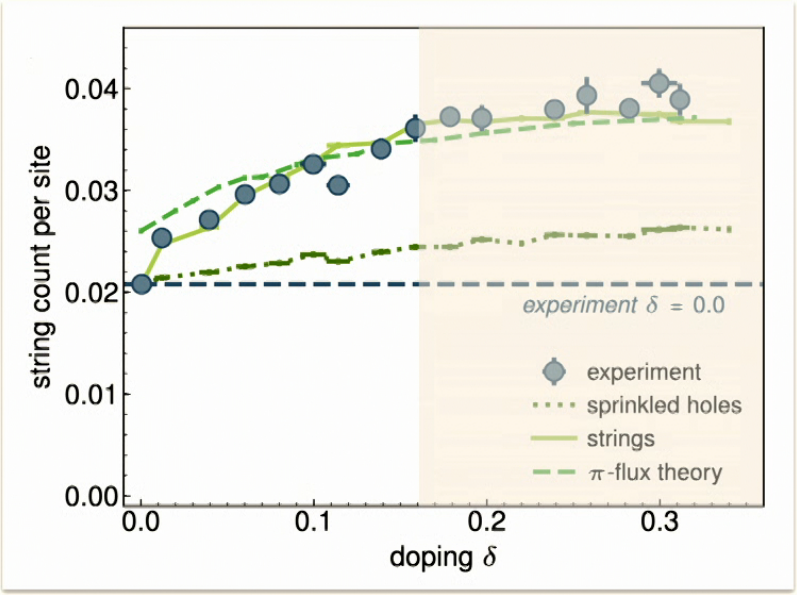

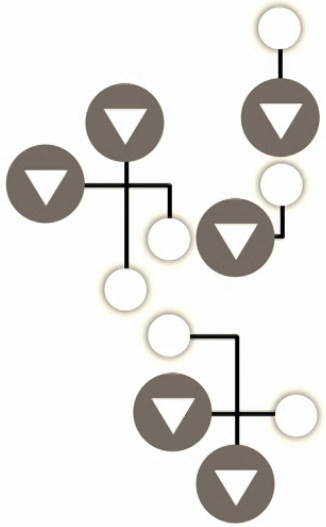

C. Chiu et al., Science 365, 6450 (2019)

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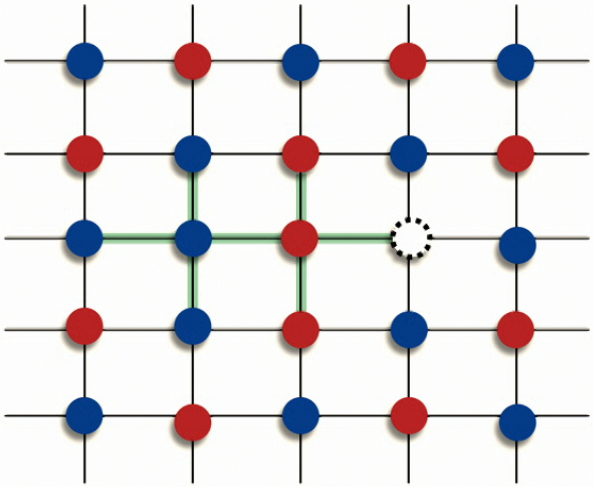
Candidate theories

Geometric string theory



Grusdt et al., PRX 8 (2018), Grusdt et al., PRB 99 (2019), Bohrdt et al., NJP 22 (2020)

Early work: Bulaevskii et al., JETP 27 (1968), Trugman, PRB 37 (1988), Manousakis, PRB 75 (2007)

Resonating valence bond theory

(π-flux theory)

$$|\psi\rangle = |\,\rangle + |\,\rangle + |\,\rangle + |\,\rangle + \ldots$$

P. W. Anderson, Science 235, 1196 (1987)

"The theoretical problem is so hard that
there isn't an obvious criterion for right."
— Steven Kivelson, Stanford University
Science 314 (2006)

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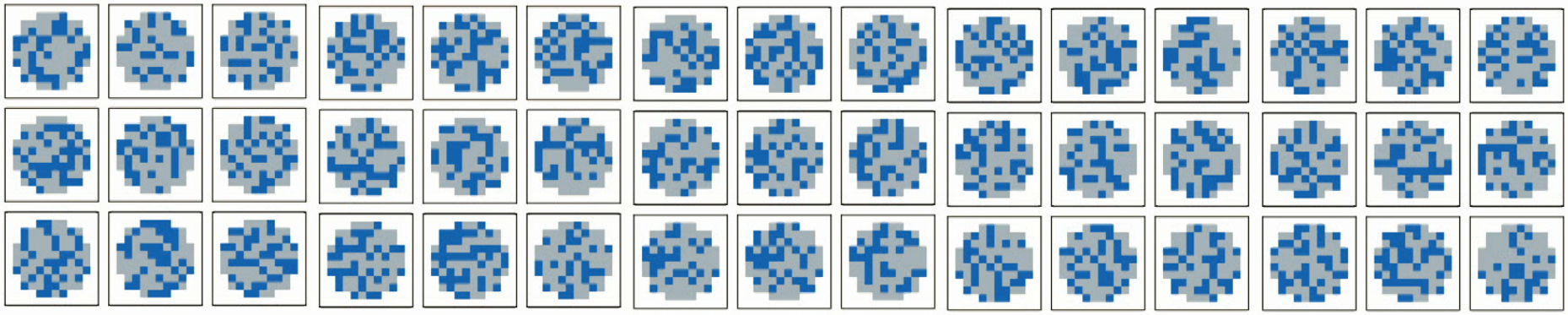

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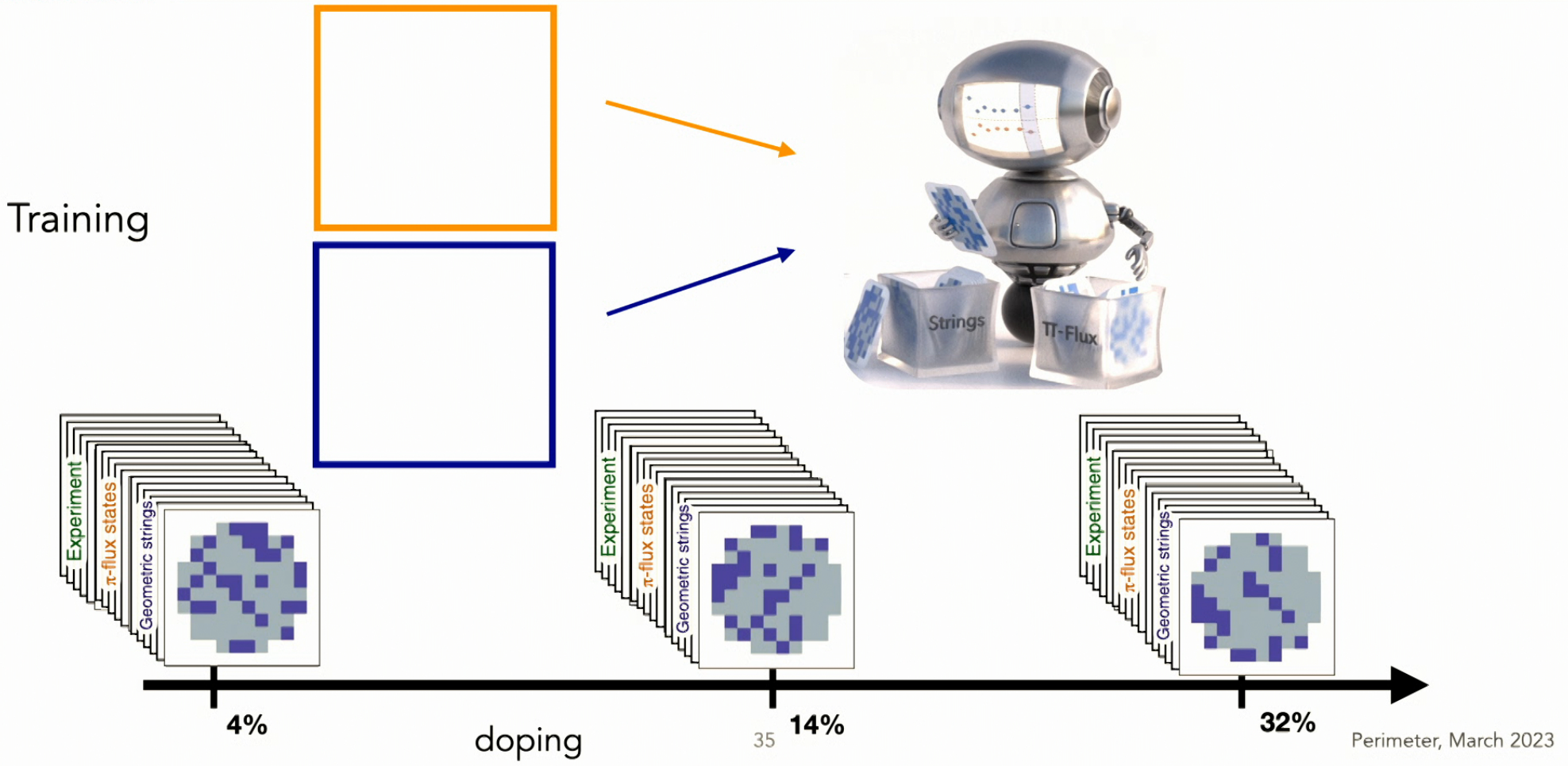
Machine learning snapshots



Perimeter, March 2023

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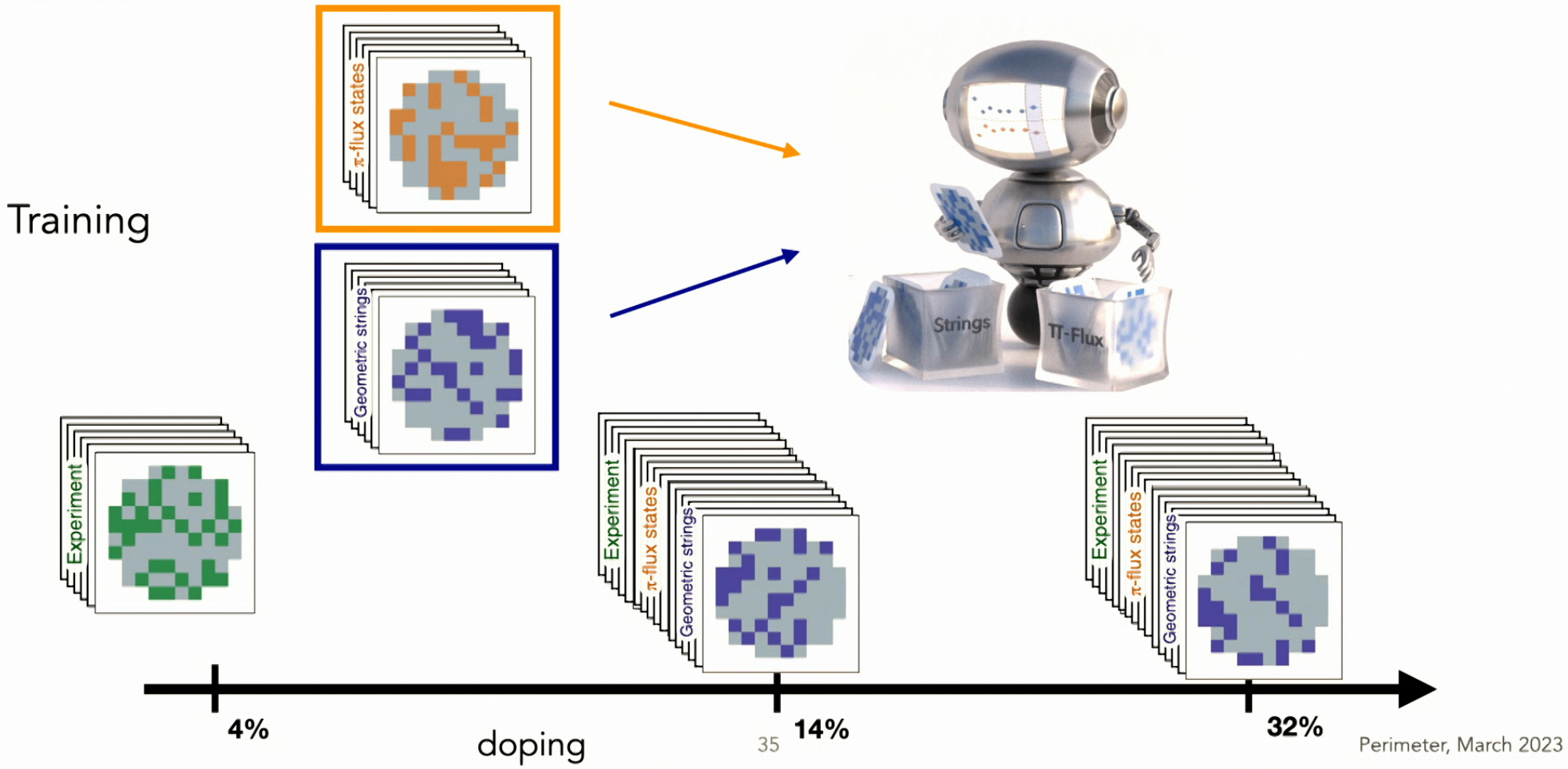
Machine learning snapshots



Perimeter, March 2023

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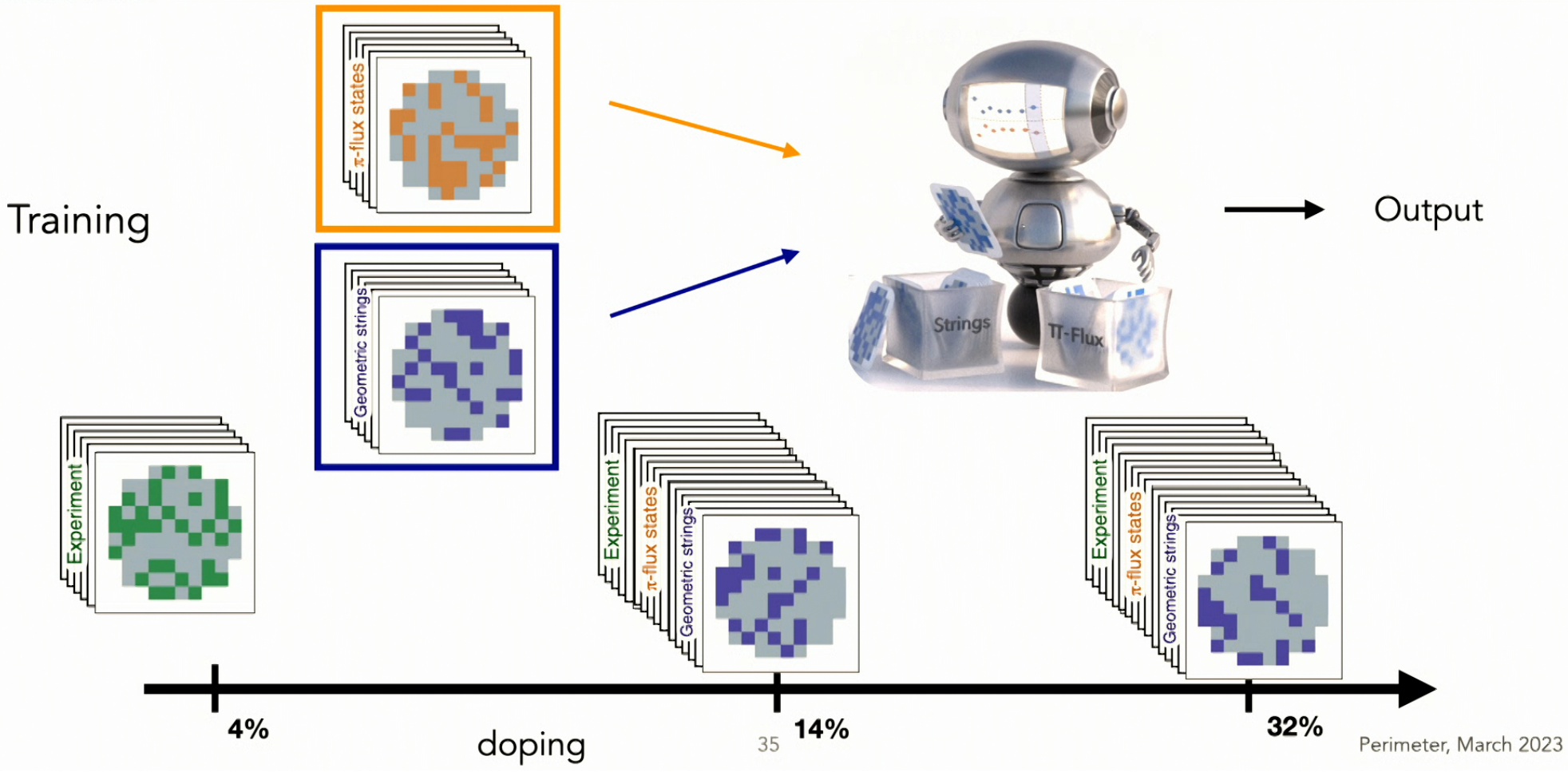
Machine learning snapshots



Perimeter, March 2023

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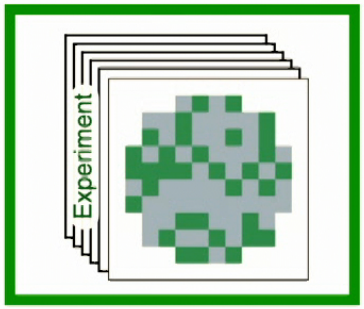
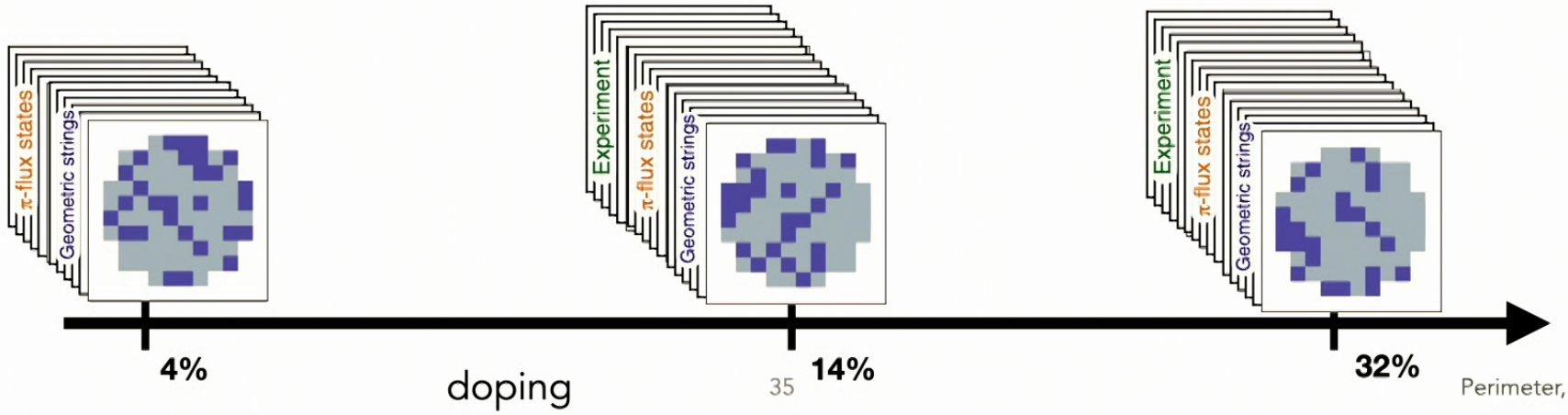
Machine learning snapshots

Classify





Perimeter, March 2023

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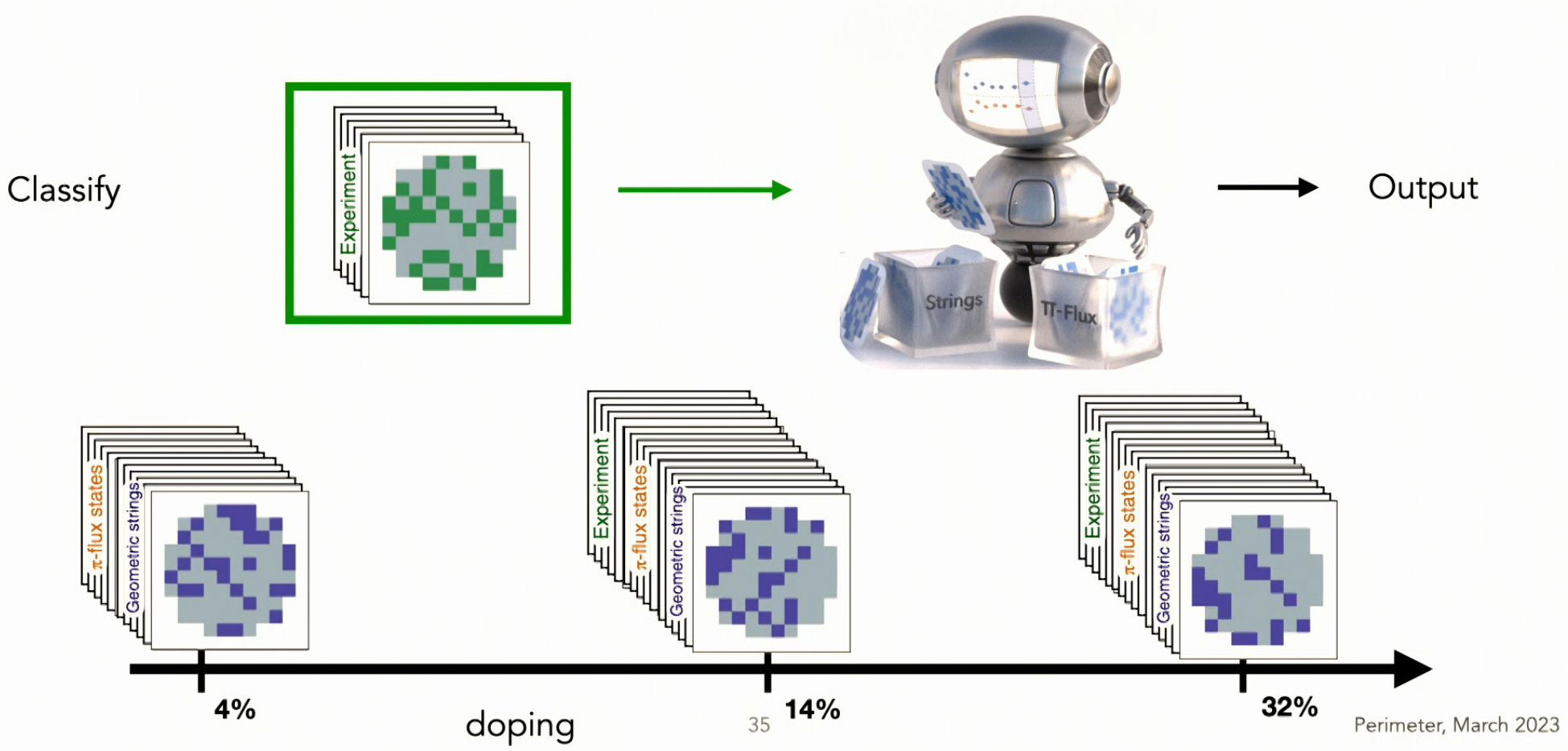
Machine learning snapshots



Perimeter, March 2023

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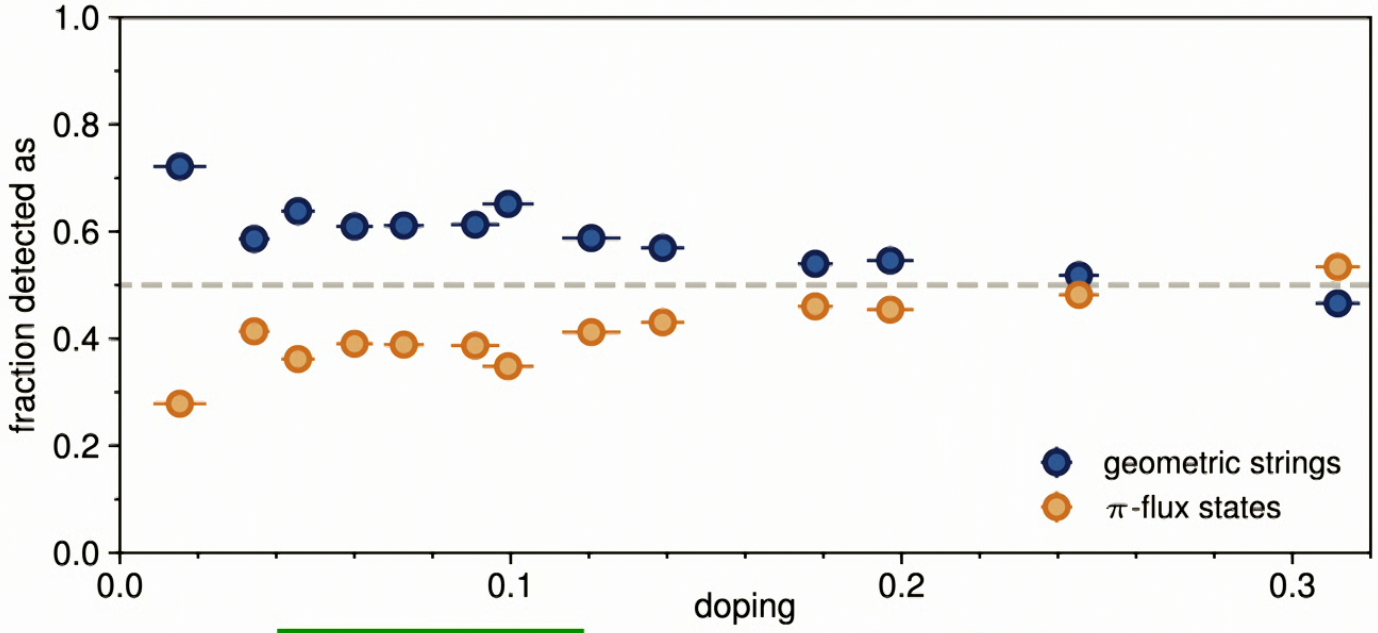
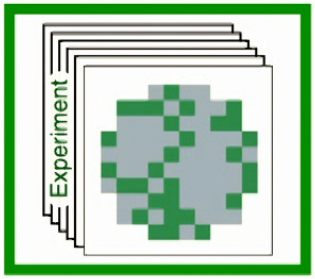


Classify



Output

Bohrdt et al., Nature Physics 15 (2019)

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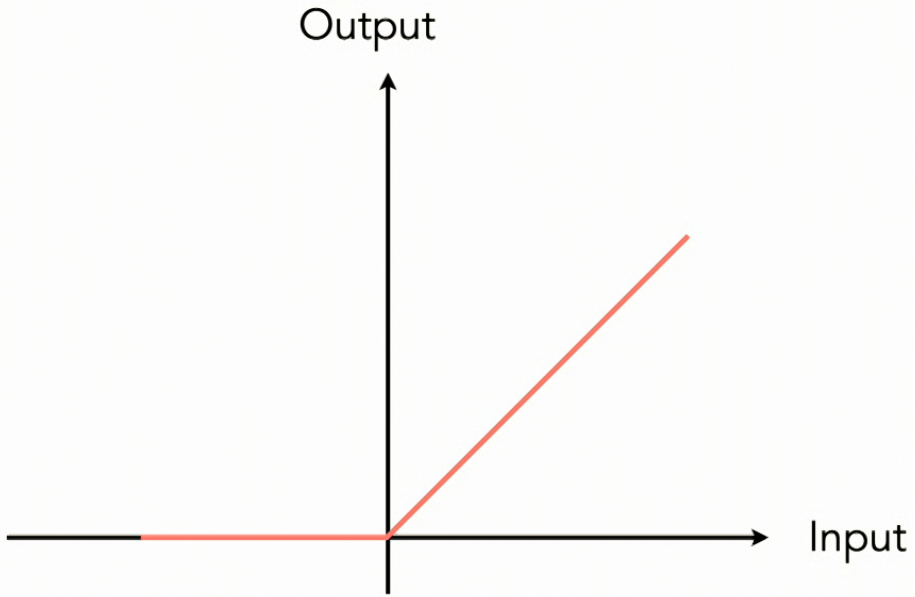
Interpretability?

- Looking at filters difficult: non-linearity mixes all orders of correlations
- Non-linearity necessary:
  otherwise, network corresponds to function that multiplies the input by a weight matrix and adds to it an additional bias vector.

Typical activation function:
rectified linear unit



Correlator convolutional neural network

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$$C_\alpha^{(1)}(\vec{x}) = \sum_{\vec{a},k} f_{\alpha,k}(\vec{a}) S_k(\vec{x}+\vec{a})$$

$$C_\alpha^{(2)}(\vec{x}) = \sum_{(\vec{a},k)\neq(\vec{b},k')} f_{\alpha,k}(\vec{a}) f_{\alpha,k'}(\vec{b}) S_k(\vec{x}+\vec{a}) S_{k'}(\vec{x}+\vec{b})$$

C. Miles, A. Bohrdt et al., Nature Communications 12, 3905 (2021)

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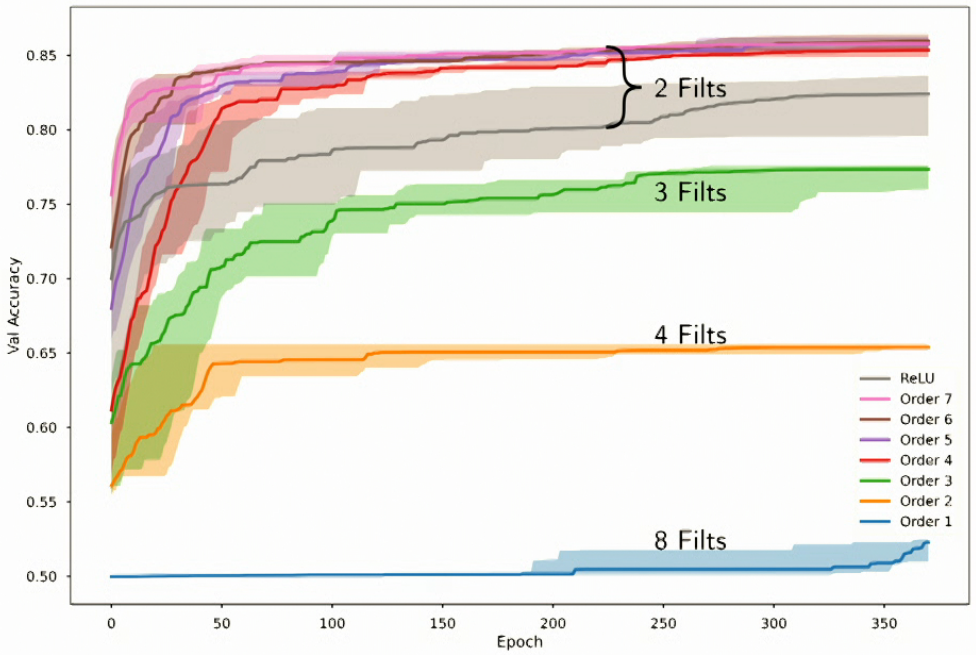
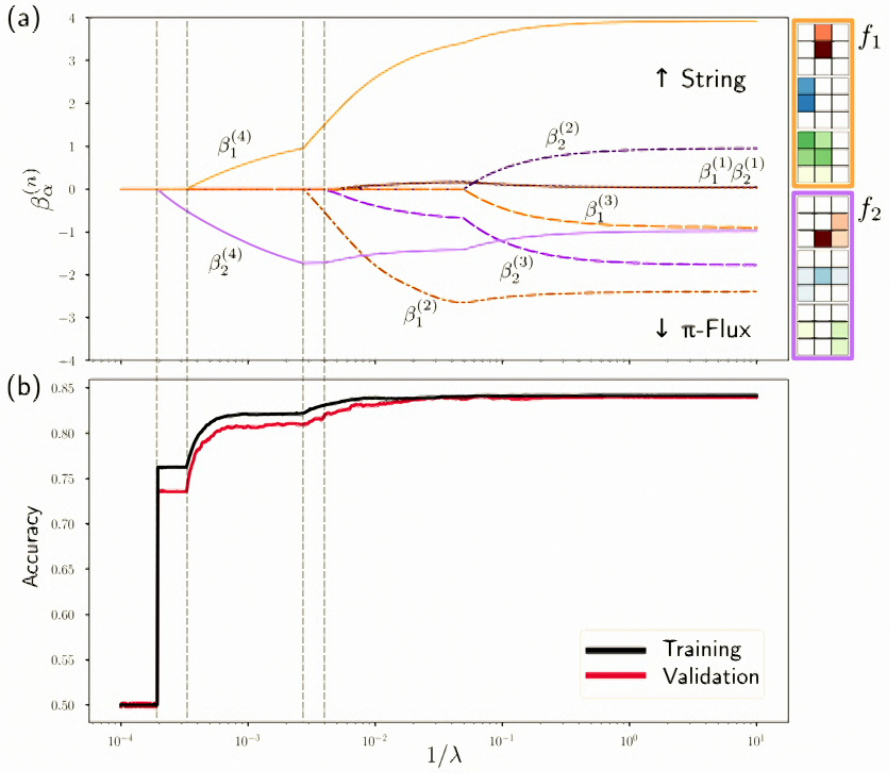
Regularization path analysis





C. Miles, A. Bohrdt et al., Nature Communications 12, 3905 (2021)

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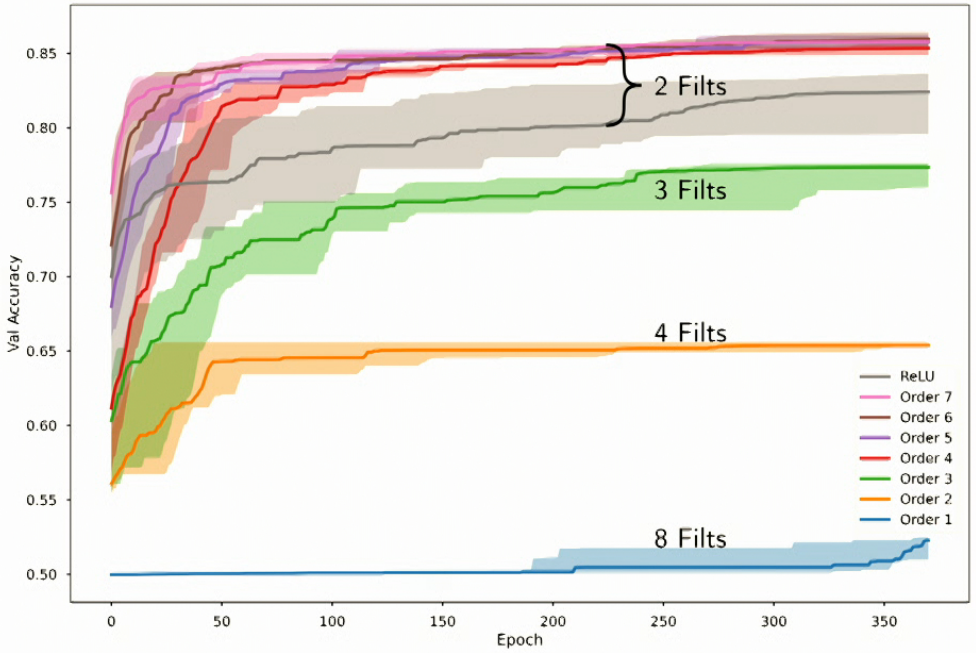
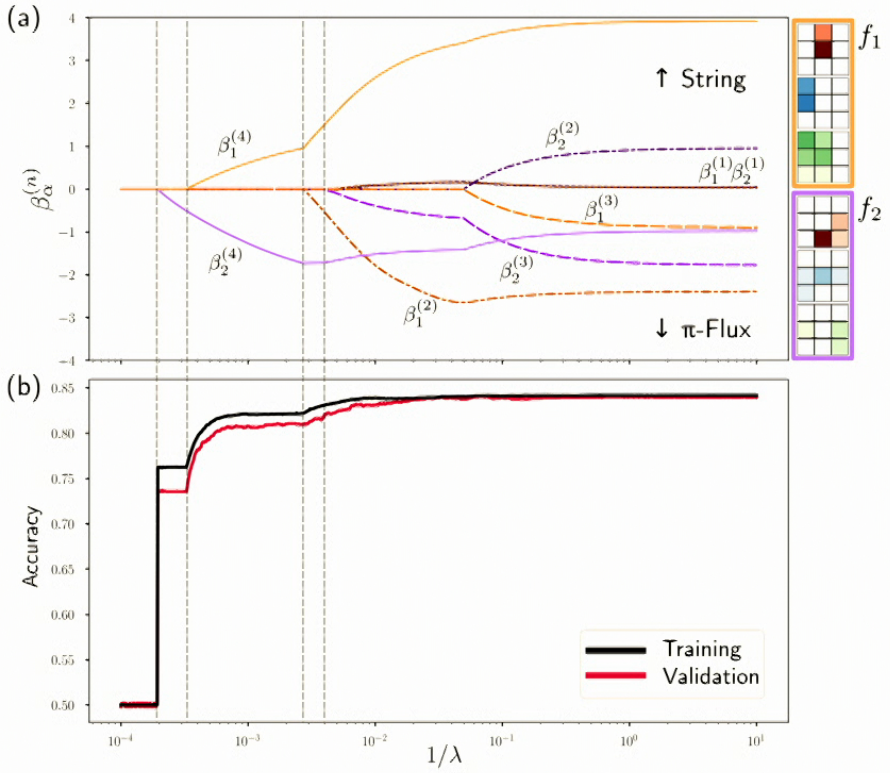
Regularization path analysis





C. Miles, A. Bohrdt et al., Nature Communications 12, 3905 (2021)

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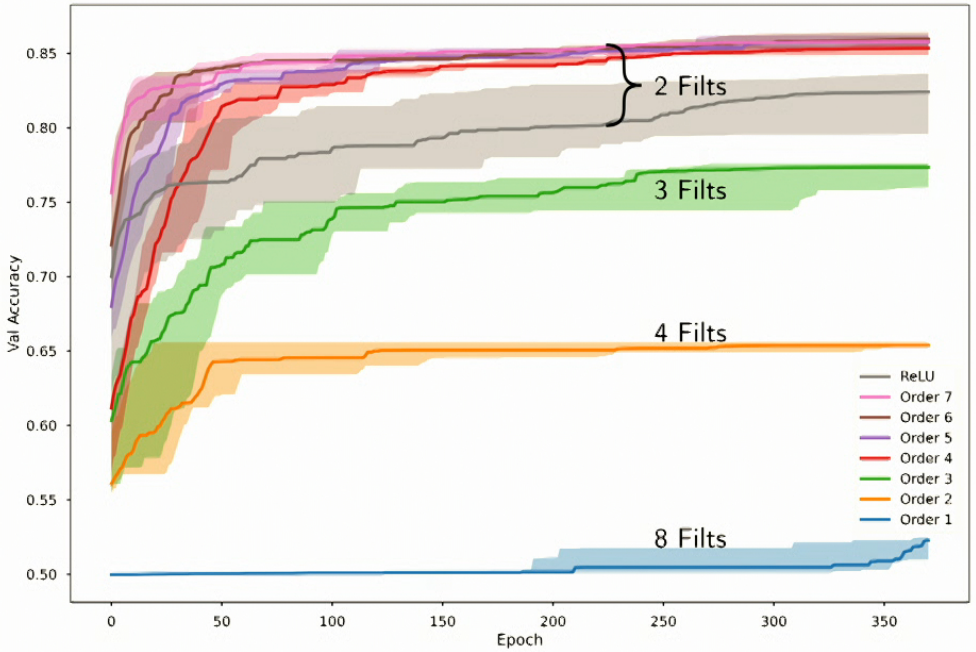
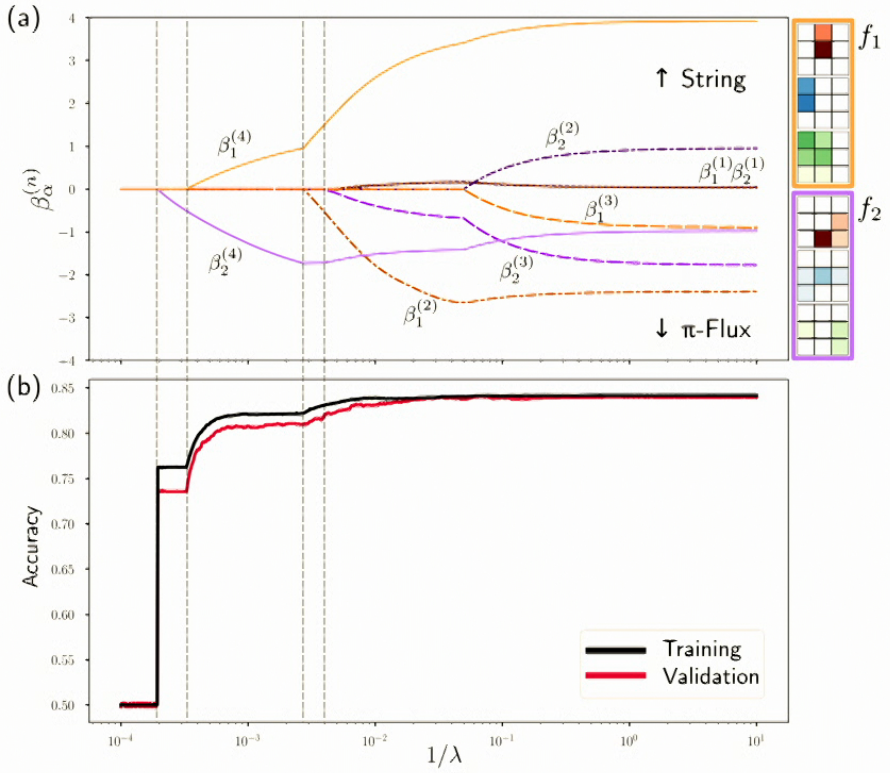
Regularization path analysis





C. Miles, A. Bohrdt et al., Nature Communications 12, 3905 (2021)

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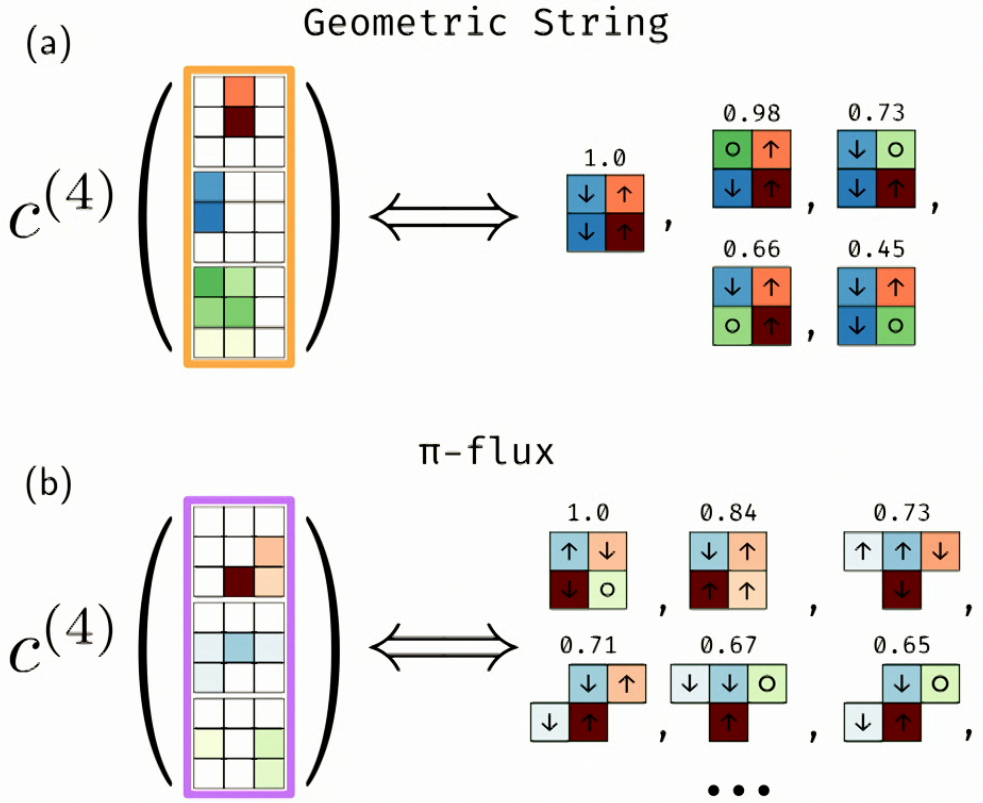
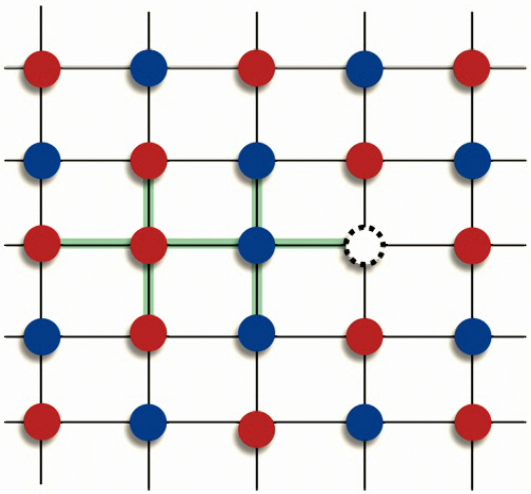
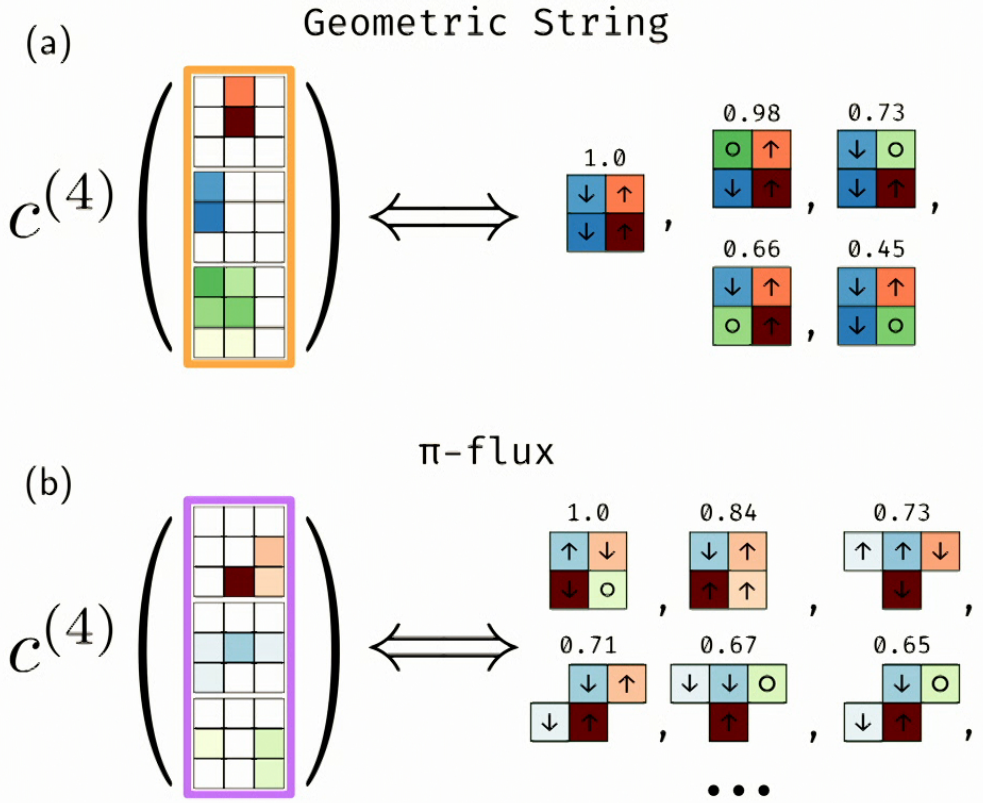
Interpretability



C. Miles, A. Bohrdt et al., Nature Communications 12, 3905 (2021)

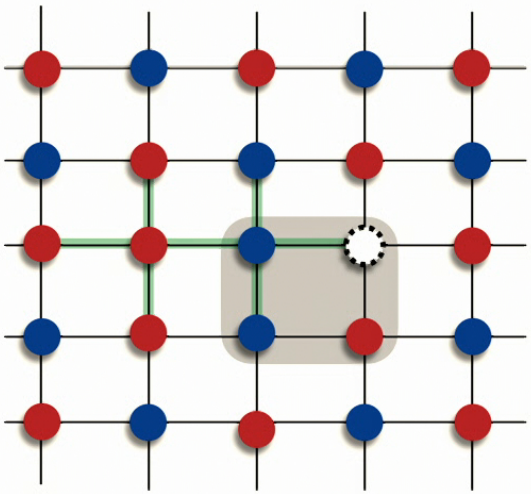
Interpretability

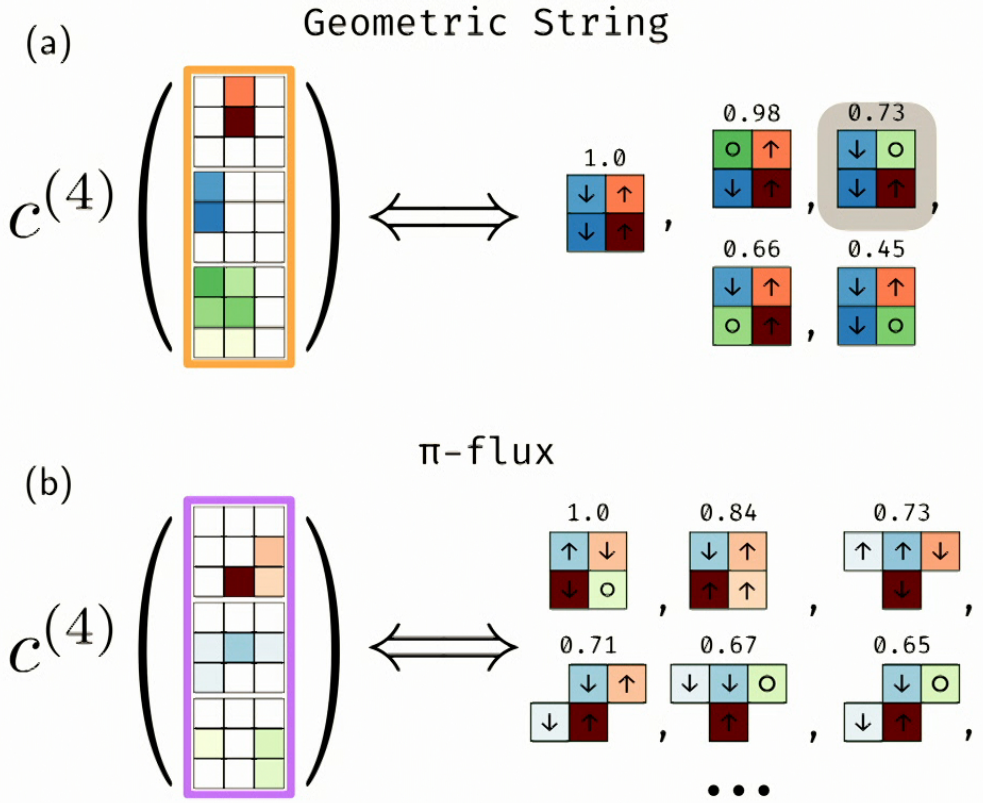




C. Miles, A. Bohrdt et al., Nature Communications 12, 3905 (2021)

Interpretability





C. Miles, A. Bohrdt et al., Nature Communications 12, 3905 (2021)

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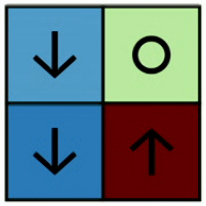
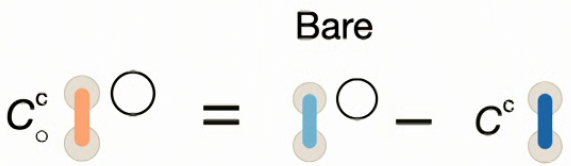
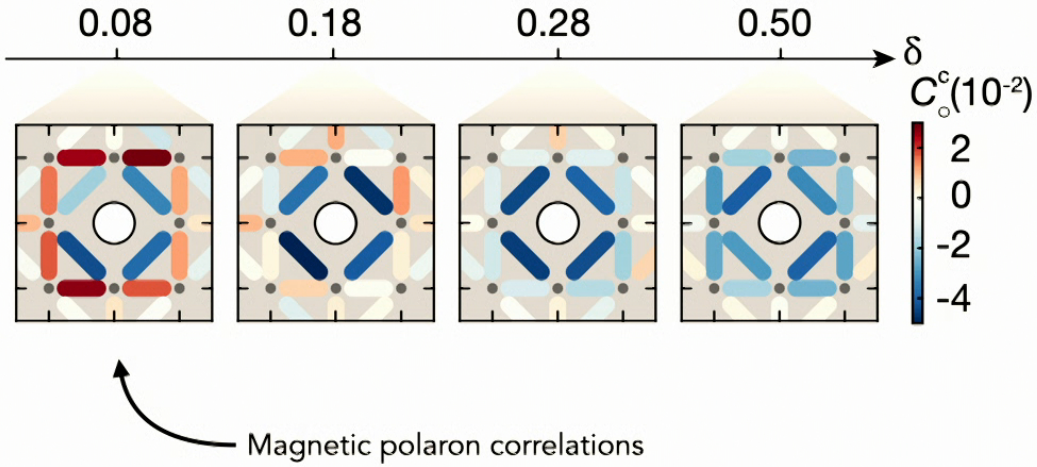
Higher-order correlations







Koepsell et al., Science 374 (2021)

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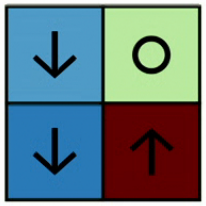
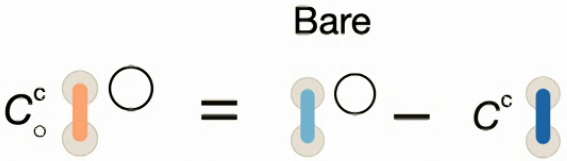
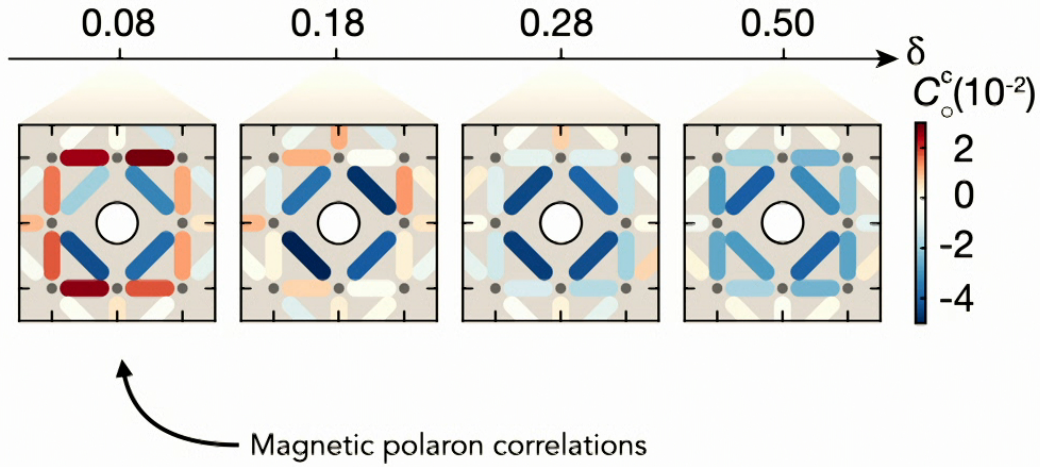
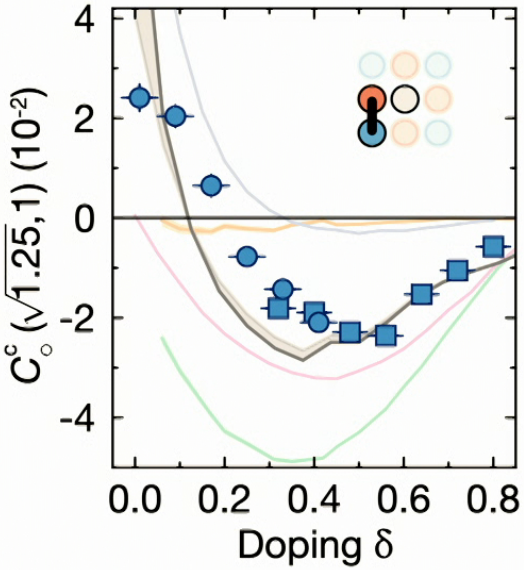
Higher-order correlations



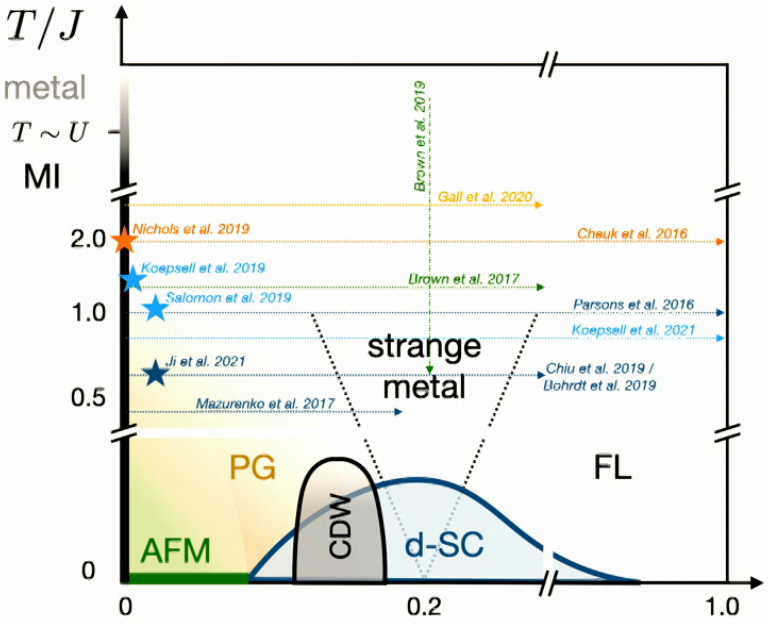




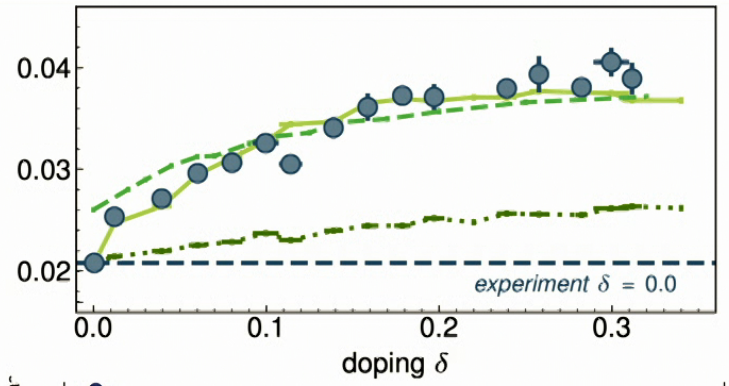


Koepsell et al., Science 374 (2021)

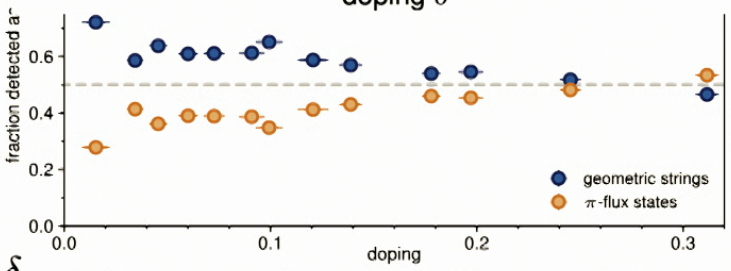
Phase diagram



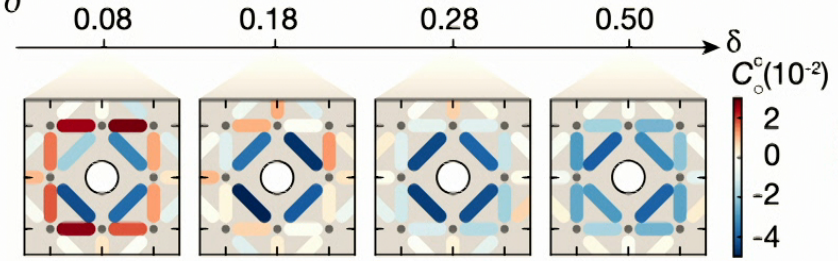
Bohrdt et al., Annals of Physics (2021)



C. Chiu et al., Science 365 (2019)



Bohrdt et al., Nature Physics 15 (2019)



Koepsell et al., Science 374 (2021)

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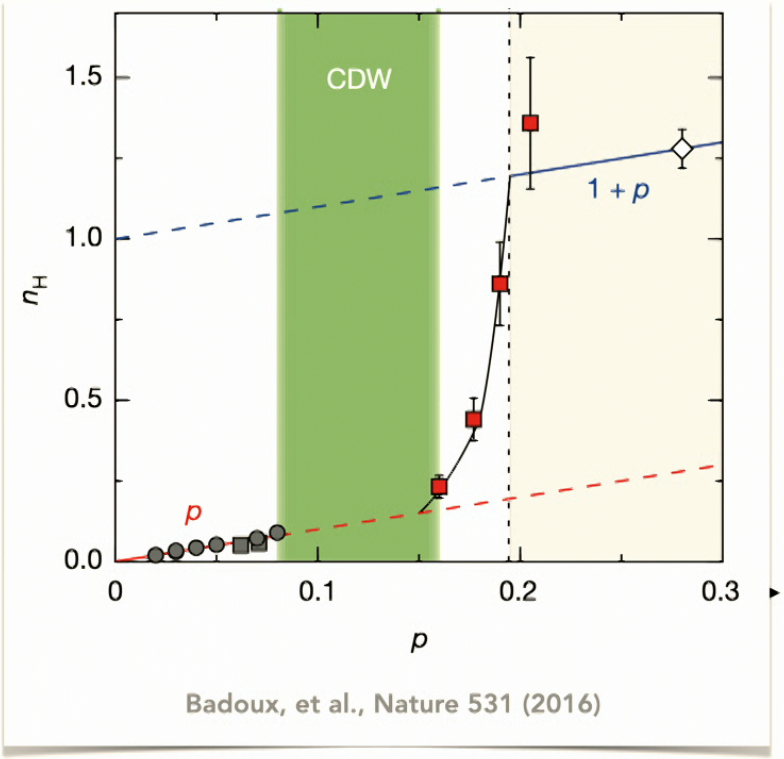
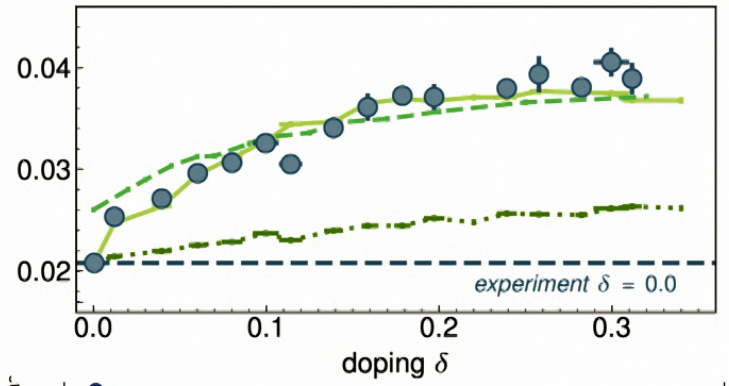
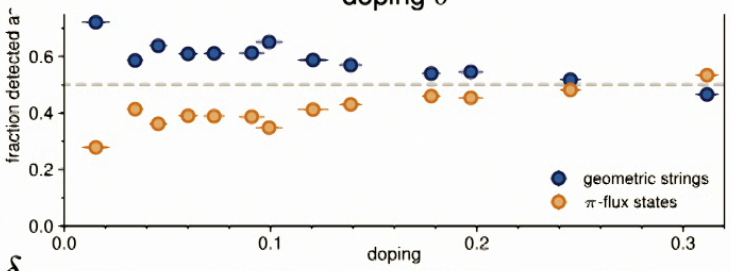
Phase diagram



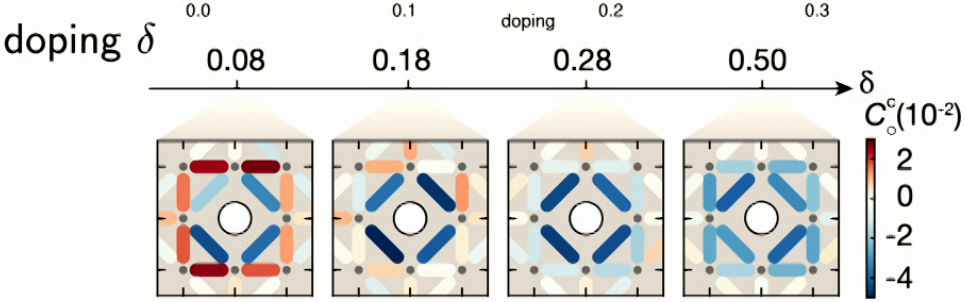
Bohrdt et al., Annals of Physics (2021)



C. Chiu et al., Science 365 (2019)



Bohrdt et al., Nature Physics 15 (2019)



Koepsell et al., Science 374 (2021)

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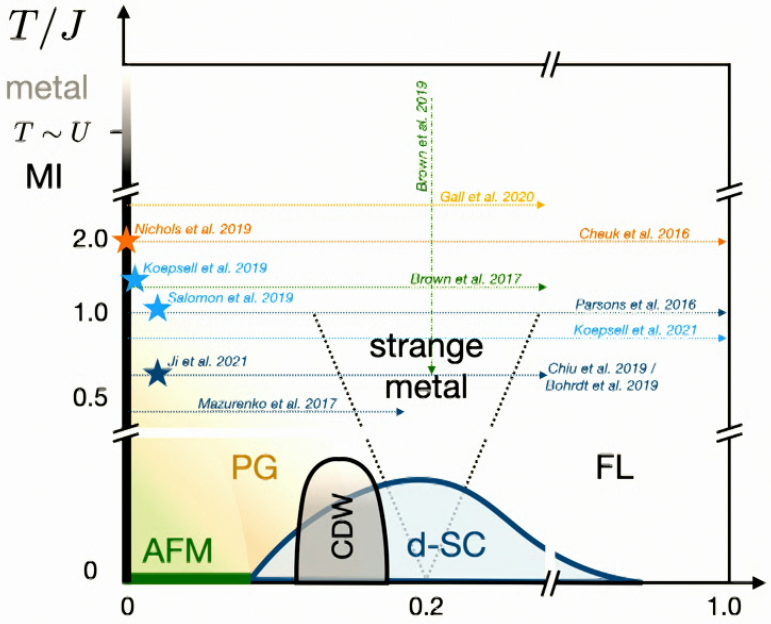
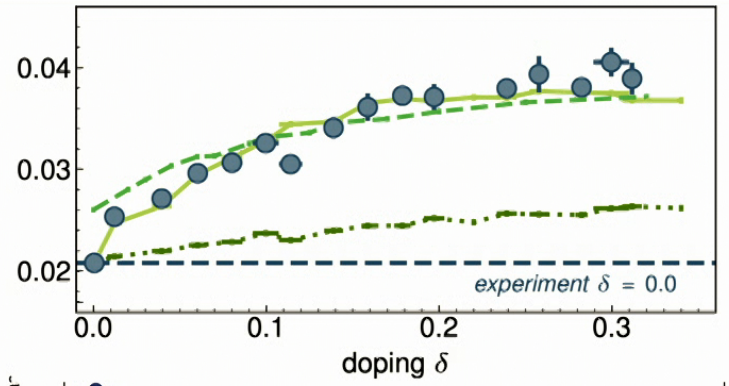


Bohrdt et al., Annals of Physics (2021)



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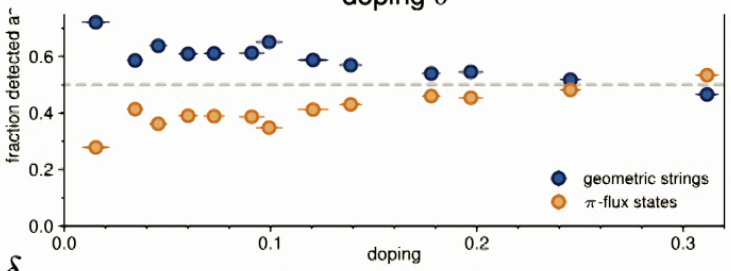

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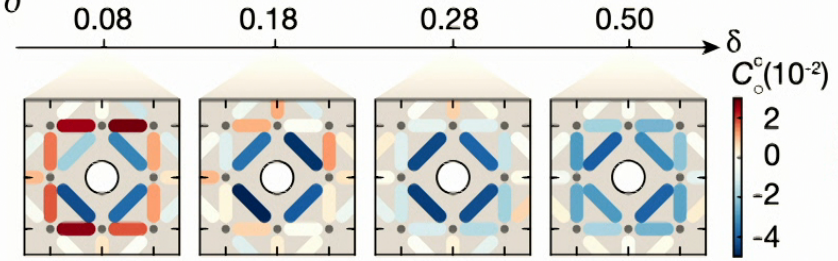

Koepsell et al., Science 374 (2021)

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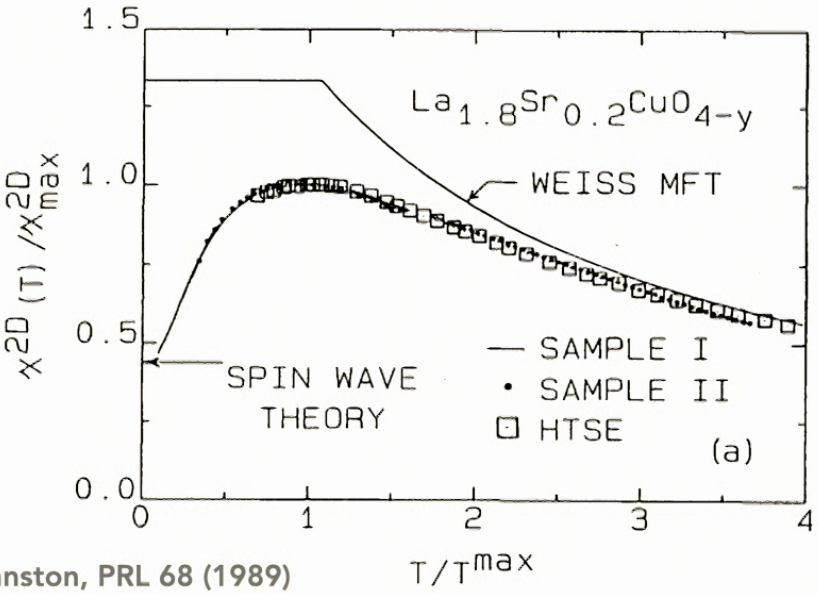
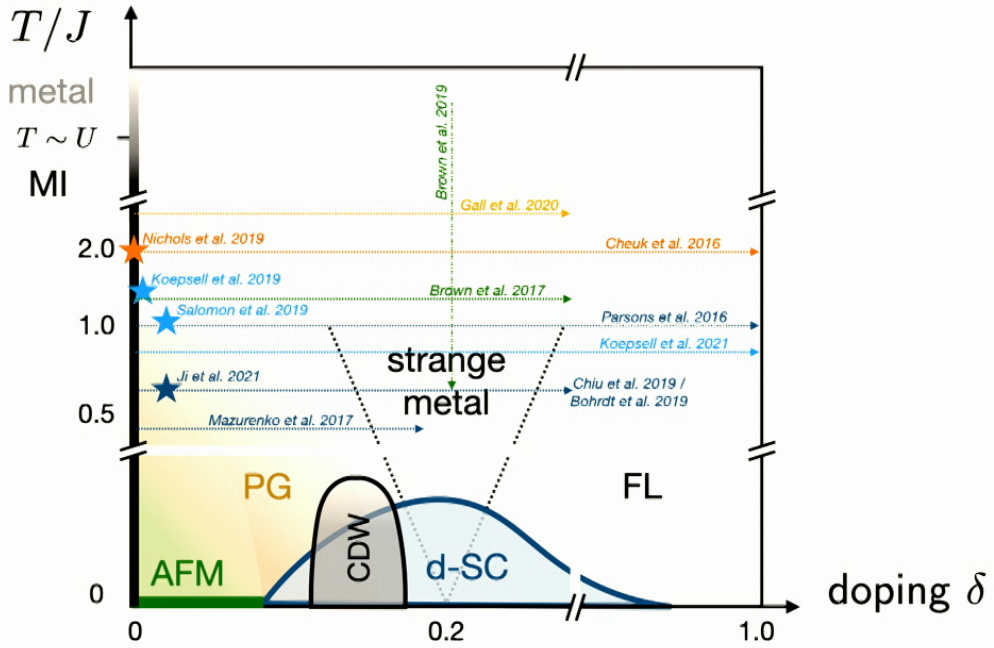
Unsupervised learning of snapshots

Measuring magnetic susceptibility



Johnston, PRL 68 (1989)



- pair state is spin singlet, suppression of spin excitations below T_c
- Preformed pairs???

Bohrdt et al., Annals of Physics (2021)

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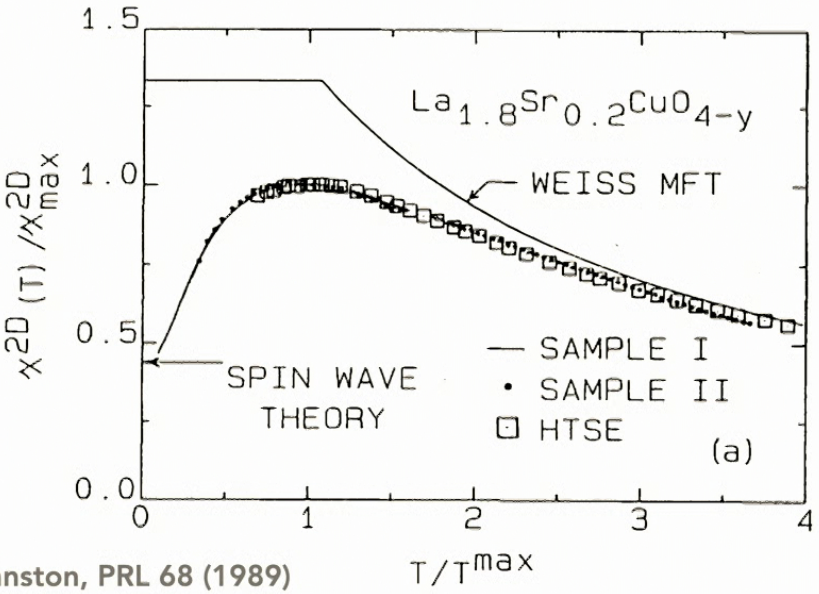
Unsupervised learning of snapshots

Measuring magnetic susceptibility



Johnston, PRL 68 (1989)

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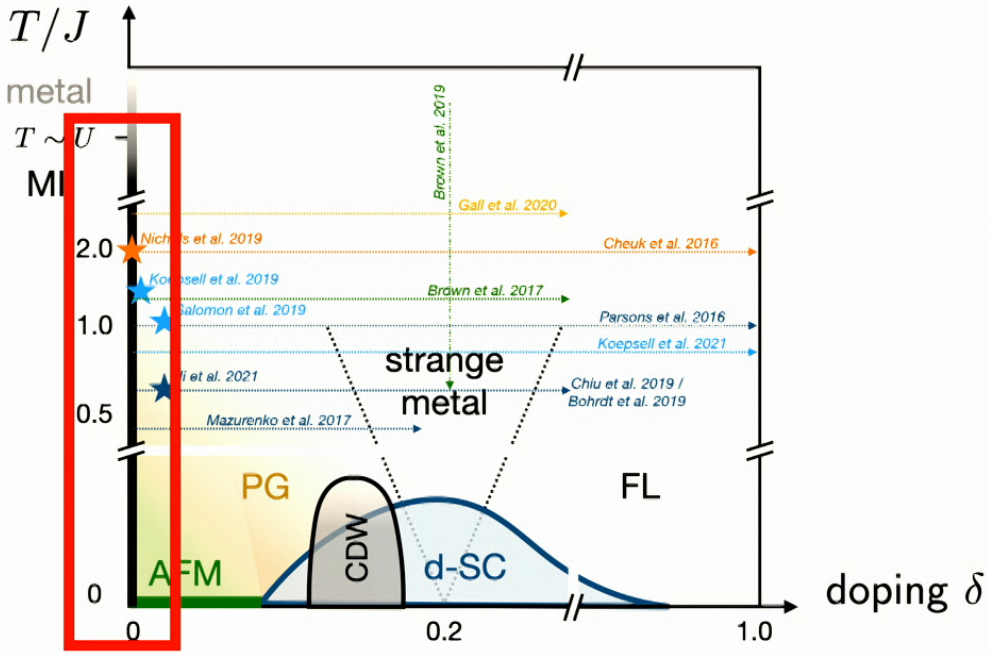
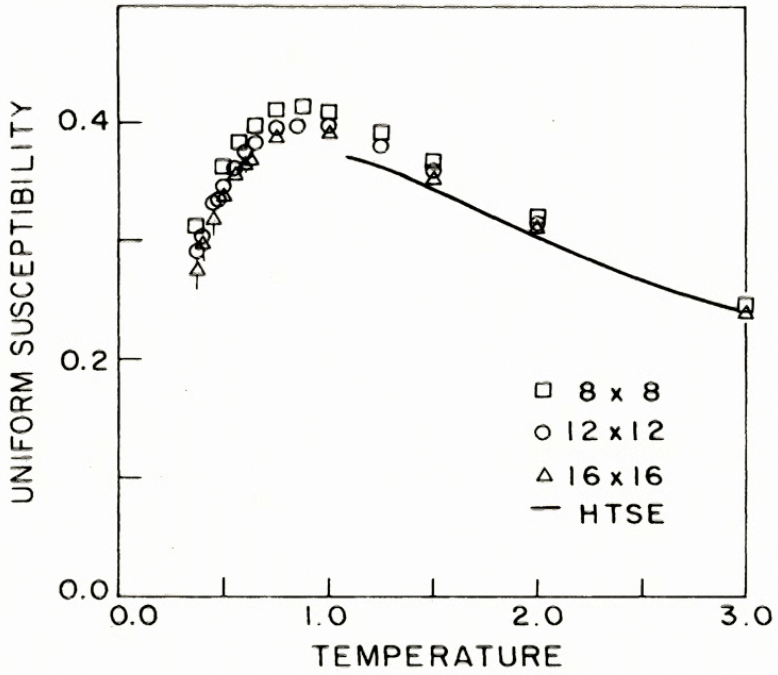


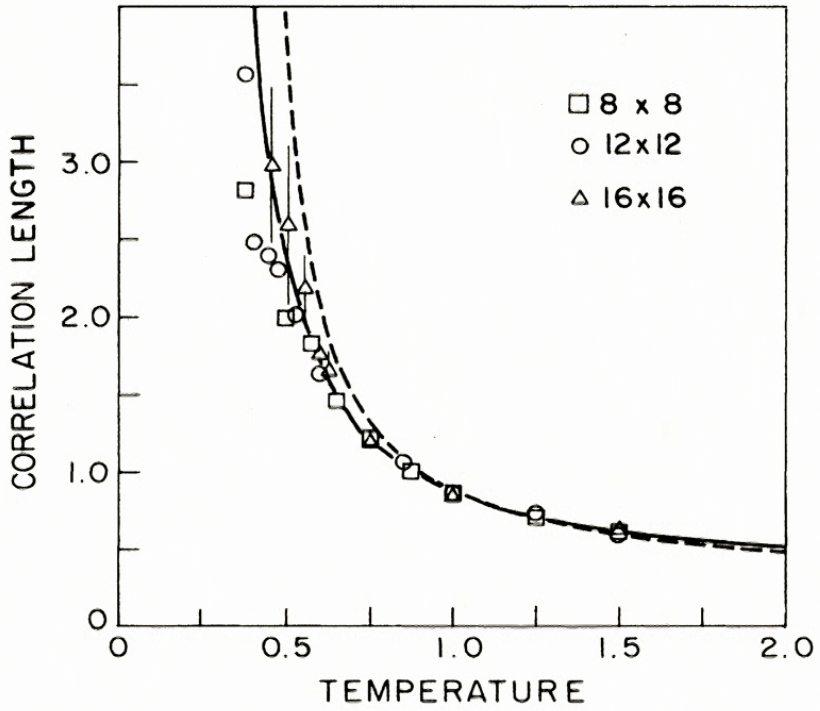
Approximate at half-filling:

Heisenberg model $\hat{H} = J \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$

Bohrdt et al., Annals of Physics (2021)

QMC for the Heisenberg model





Gomez-Santos et al., PRB 39 (1989)

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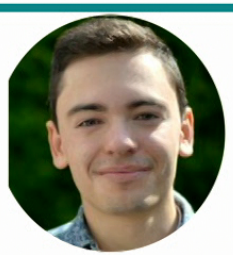
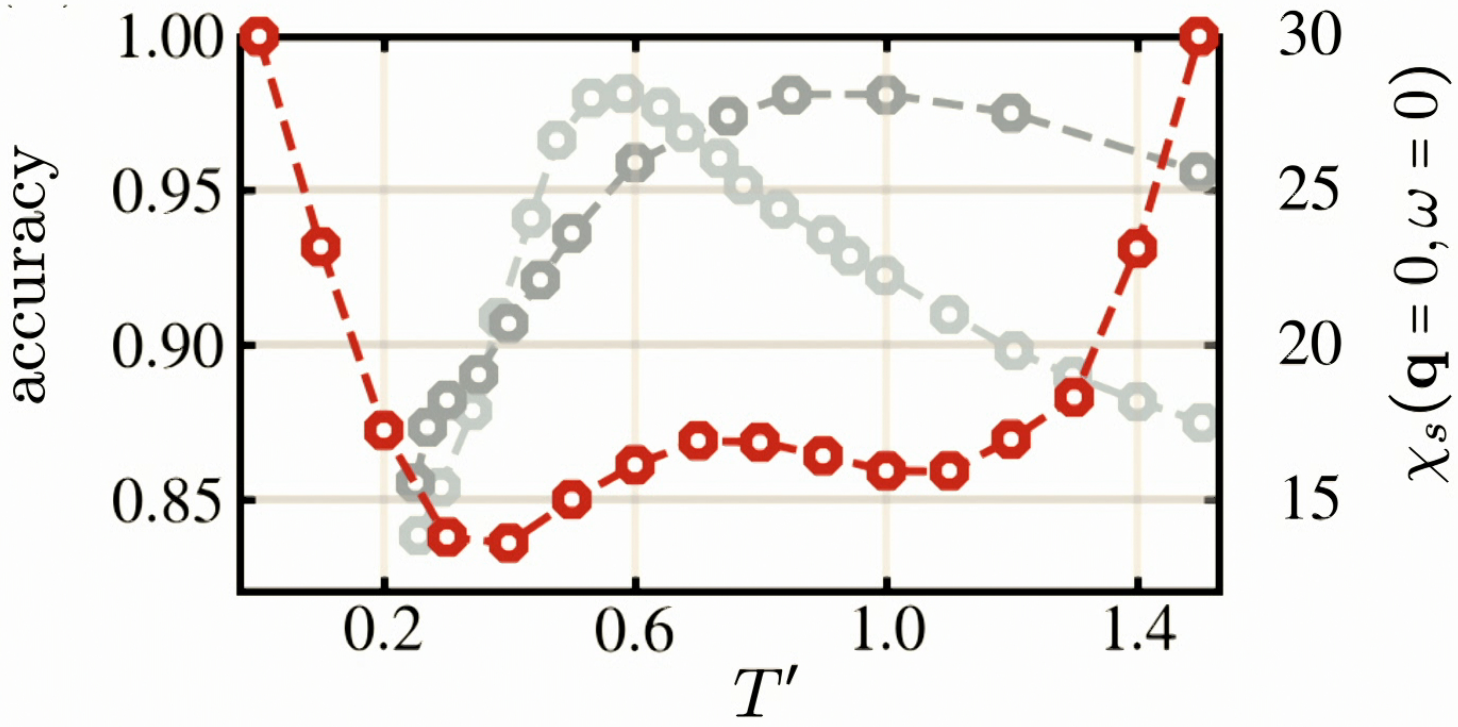
Confusion learning Heisenberg snapshots





Schlömer et al., arXiv2303.XXXX

Introduced in van Nieuwenburg et al., Nature Physics, 13 (2017)

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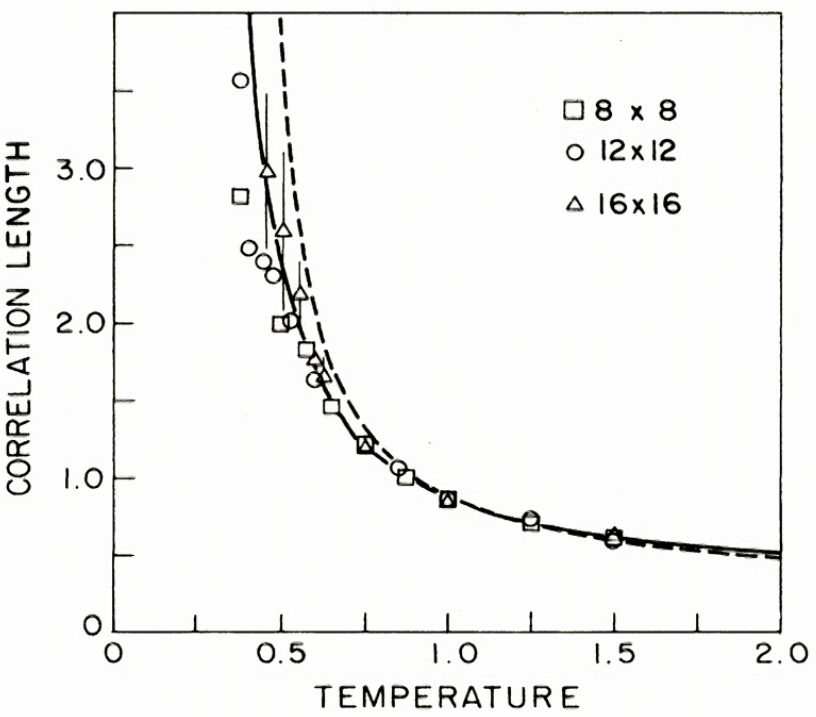
Interpretability



Gomez-Santos et al., PRB 39 (1989)

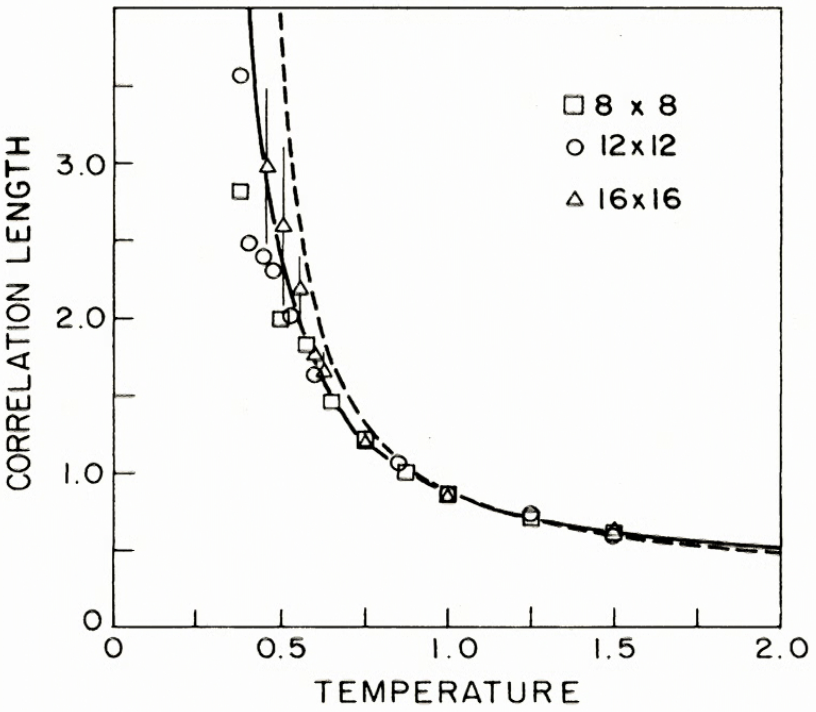
$$\sigma^2_{c_1} = \left\langle \left(\sum_{i,e} \hat{S}^z_i \hat{S}^z_{e_i} \right)^2 \right\rangle - \left\langle \sum_{i,e} \hat{S}^z_i \hat{S}^z_{e_i} \right\rangle^2$$

$$= \sum_{i,j,e_i,e_j} \left\langle \hat{S}^z_i \hat{S}^z_{e_i} \hat{S}^z_j \hat{S}^z_{e_j} \right\rangle - \left\langle \sum_{i,e} \hat{S}^z_i \hat{S}^z_e \right\rangle^2$$

Schlömer et al., arXiv2303.XXXX

Annabelle Bohrdt

Interpretability



Gomez-Santos et al., PRB 39 (1989)

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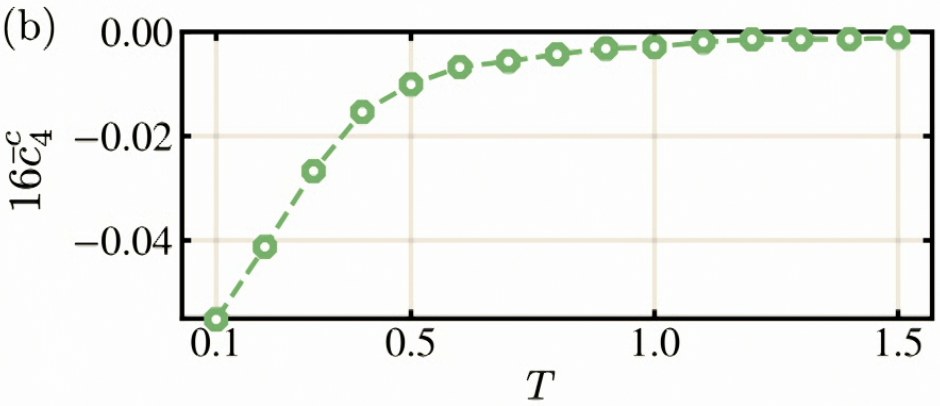
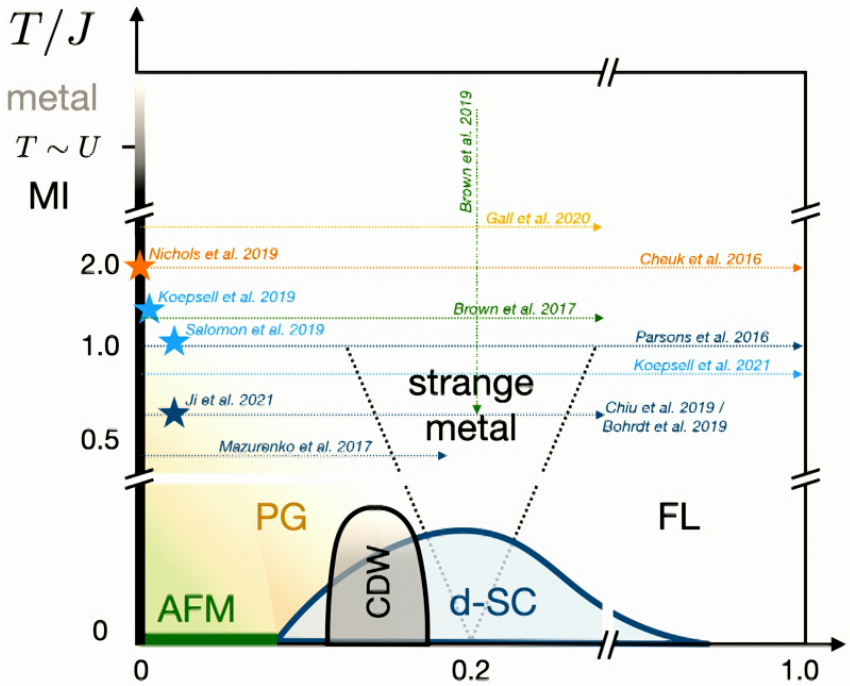
Connected 4 point c1-c1 correlator



Schlömer et al., arXiv2303.XXXX

Annabelle Bohrdt

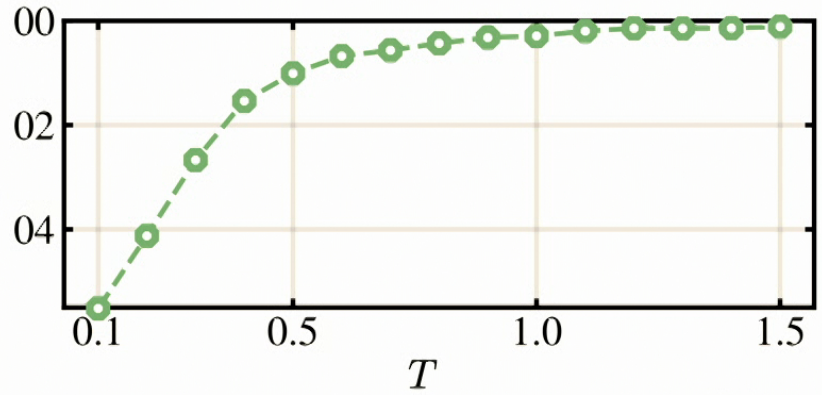
Interpretability



$$\sigma^2 = \left\langle \left(\sum_{i,e} \hat{S}^z_i \hat{S}^z_{e_i} \right)^2 \right\rangle - \left\langle \sum_{i,e} \hat{S}^z_i \hat{S}^z_{e_i} \right\rangle^2$$

$$= \sum_{i,j,e_i,e_j} \left\langle \hat{S}^z_i \hat{S}^z_{e_i} \hat{S}^z_j \hat{S}^z_{e_j} \right\rangle - \left\langle \sum_{i,e} \hat{S}^z_i \hat{S}^z_e \right\rangle^2$$

Connected 4 point c1-c1 correlator



Bohrdt et al., Annals of Physics (2021)

Schlömer et al., arXiv2303.XXXX

Numerics Review from last year:

2. Phase diagram and phase boundaries

Not much is known about the precise phase diagram of the Hubbard model in two dimensions. While the ground-state phase diagram of the model at weak coupling is fairly well understood (49, 266), the phase diagram in the intermediate-to-strong interaction limit is hotly debated. Determining precise phase boundaries is hindered by the fact that the diver-

Qin et al., Annual Review of Condensed Matter Physics 13 (2022)

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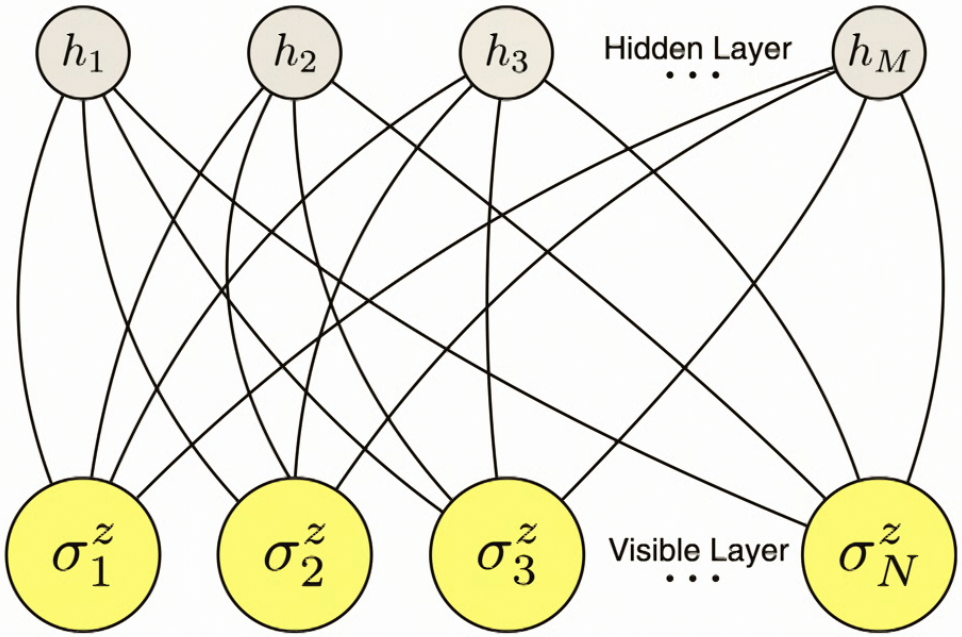
Neural network quantum states for fermions

Represent (complex) quantum states with neural networks:

Carleo & Troyer, 2017
Hibat-Allah et al., 2020
Roth et al., 2020
Hibat-Allah et al. 2022
...



Carleo & Troyer, Science 355 (2017)

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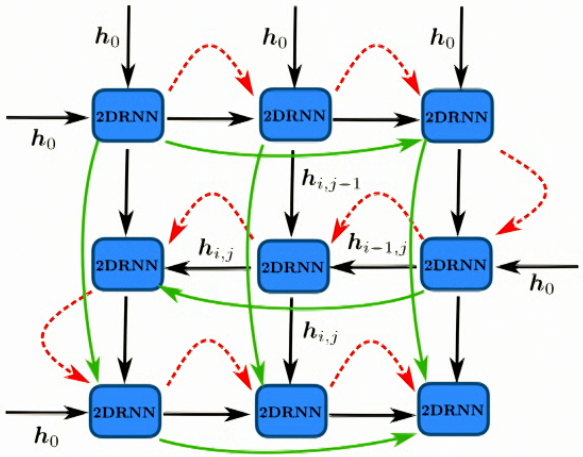

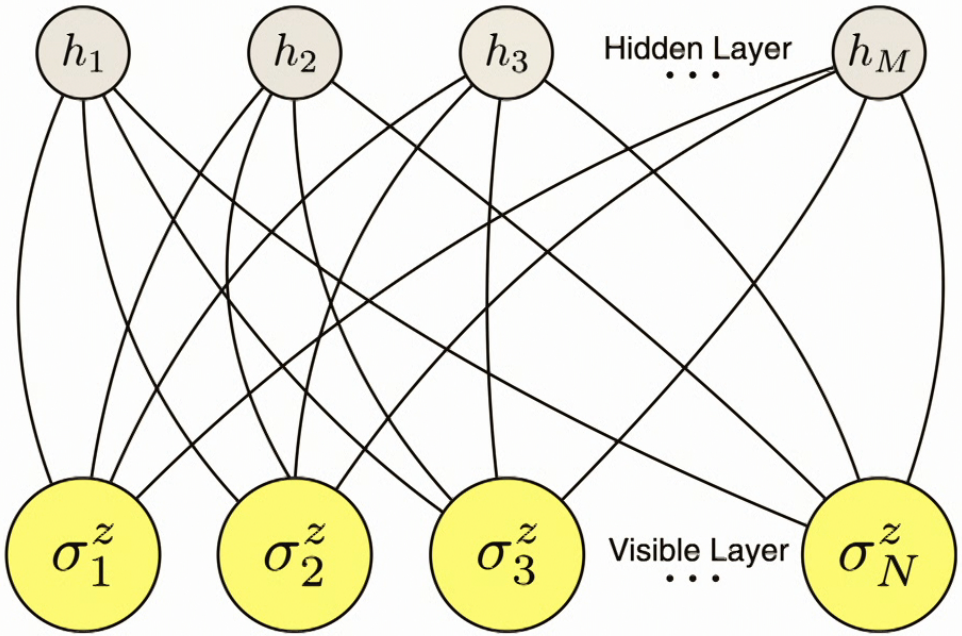

Carleo & Troyer, Science 355 (2017)

Hibat-Allah et al., arXiv:2303.11207

Neural network quantum states for fermions

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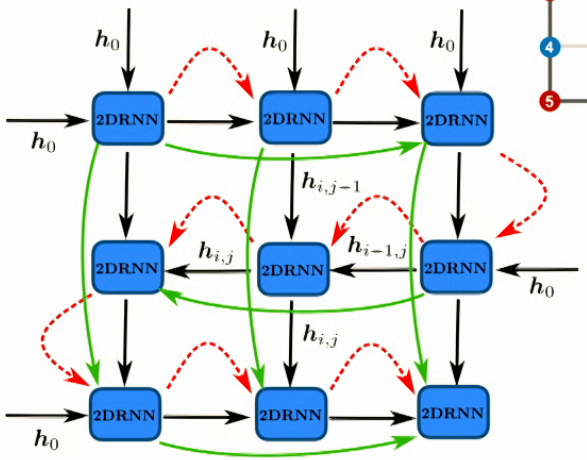
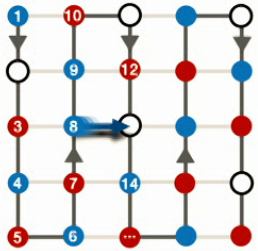


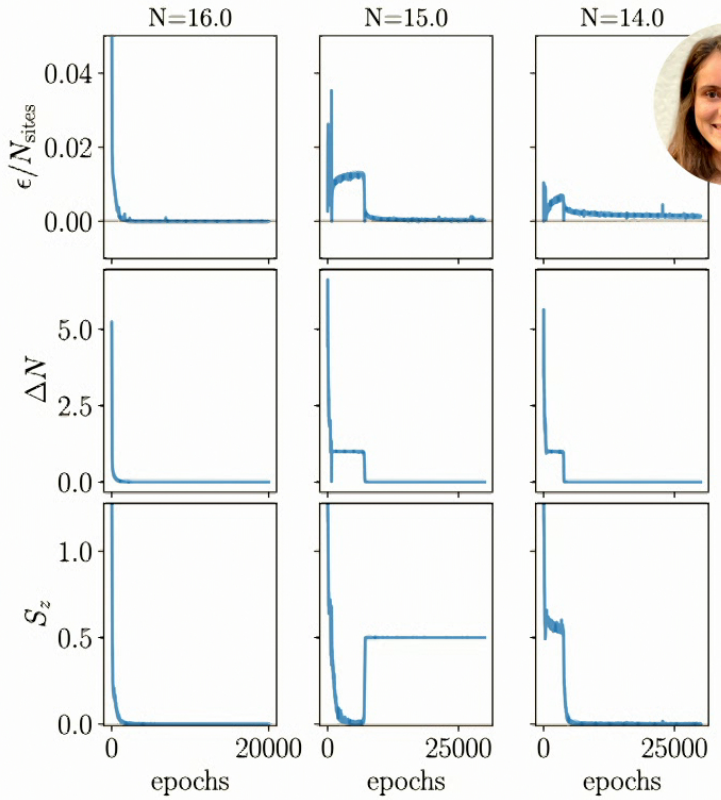


Energies

$$\epsilon = \frac{|E_{ED} - E_{RNN}|}{|E_{ED}|}$$

Particle Number

Total Magnetization



Lange et al., arXiv2304.XXXX

Hibat-Allah et al., arXiv:2303.11207

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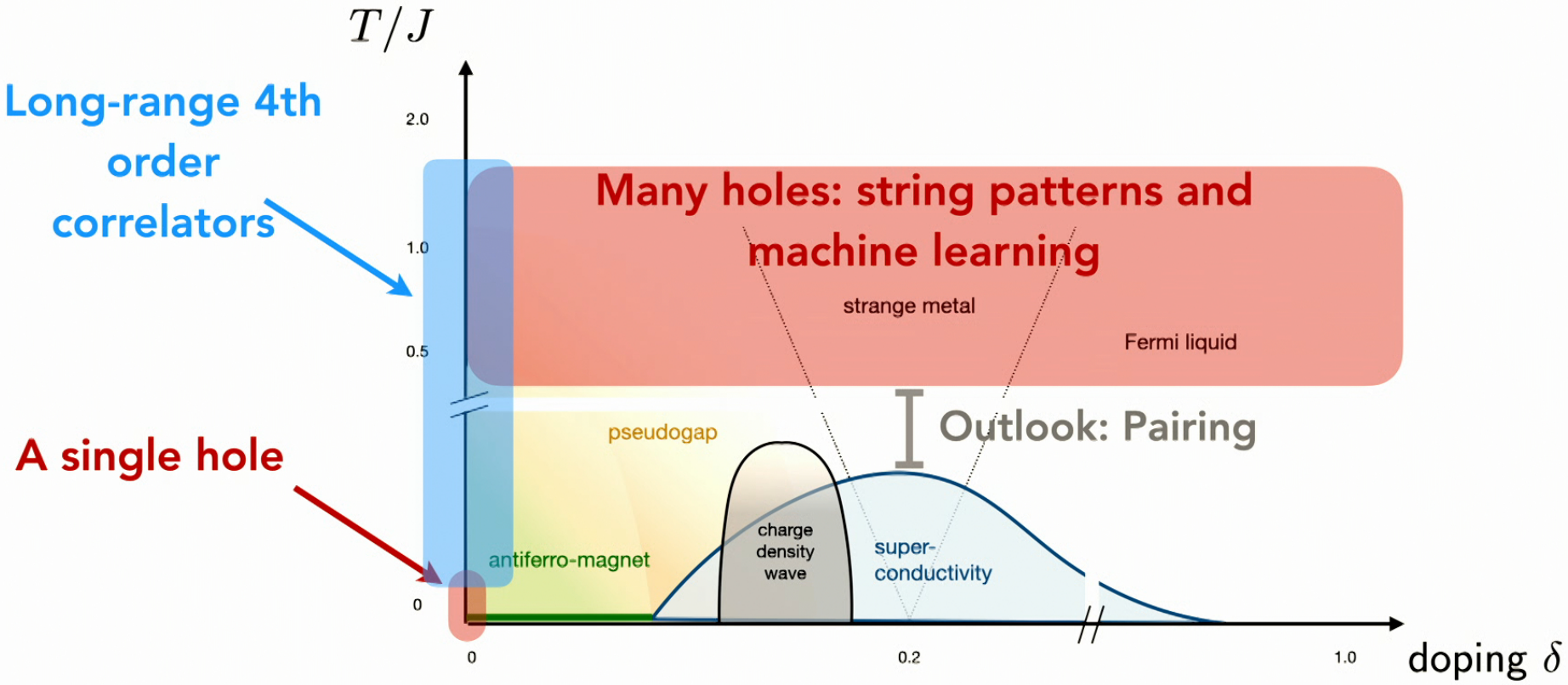
Summary



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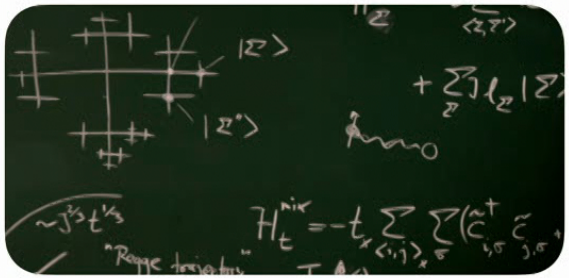
Outlook



- Microscopic models with strong pairing or robust stripes

Bohrdt et al., Nature Physics (2022)
Schlömer et al., arXiv 2208.07366
Hirthe et al., Nature (2023)

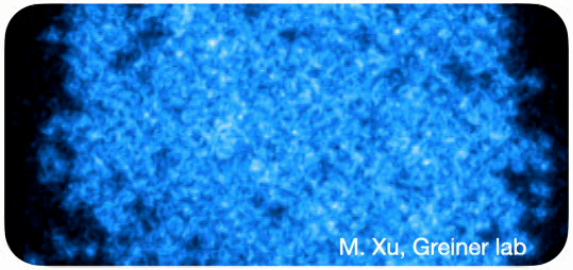
- Pairing symmetry & signatures of pairs

Bohrdt et al., arXiv:2210.02322
Grusdt et al., arXiv:2210.02321

- Neural network states for fermionic systems

Lange et al., arXiv2304.XXXX

- Large 2D systems, Fermi-Hubbard model, other geometries



- Pseudogap signatures from snapshots

Schlömer et al., arXiv2303.XX

- Application at finite doping, experimental data

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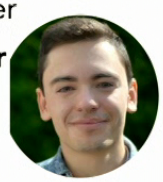
Thank you for your attention!

Hannah Lange

Fabian Döschl
Tizian Blatz
Christian Reinmoser
Henning Schlömer



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