Machine learning quantum phases of matter

Summer School on Emergent Phenomena in Quantum Materials
Cornell, May 2017

Simon Trebst
University of Cologne

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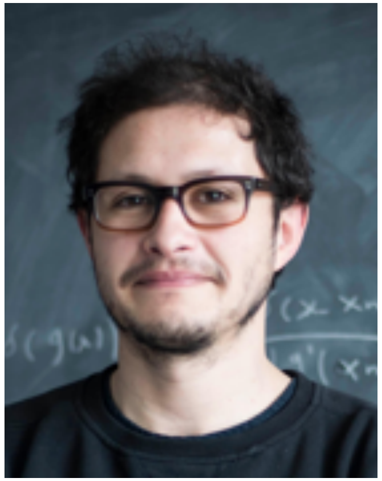
Collaborators



Juan Carrasquilla

Roger Melko

Waterloo / Perimeter

Peter Bröcker

Cologne

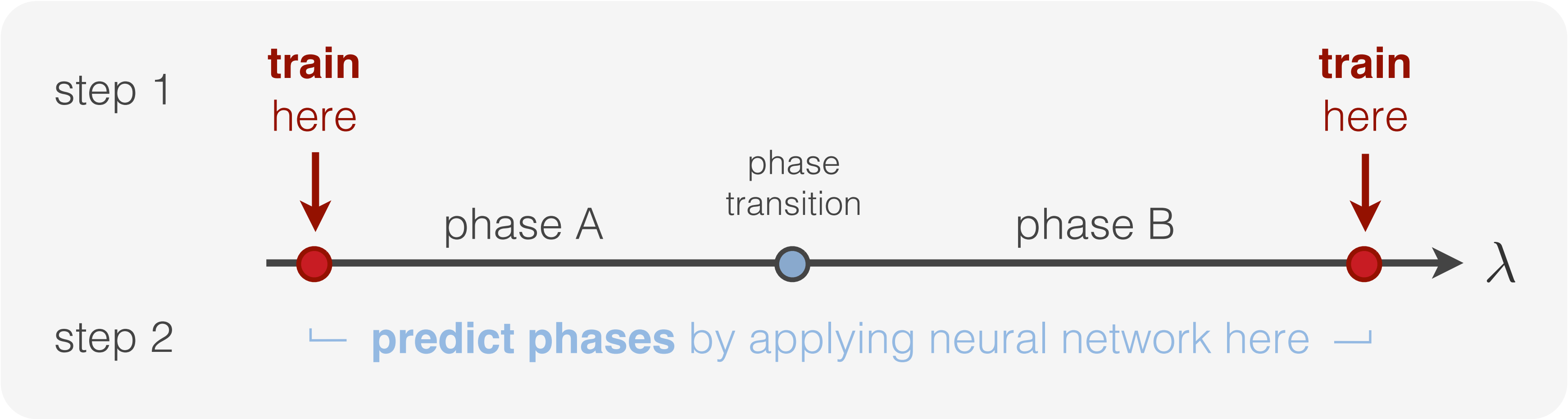
Fakher Assaad

Würzburg

Supervised learning approach

General setup

Consider some Hamiltonian, which as a function of some parameter λ exhibits a phase transition between two phases.

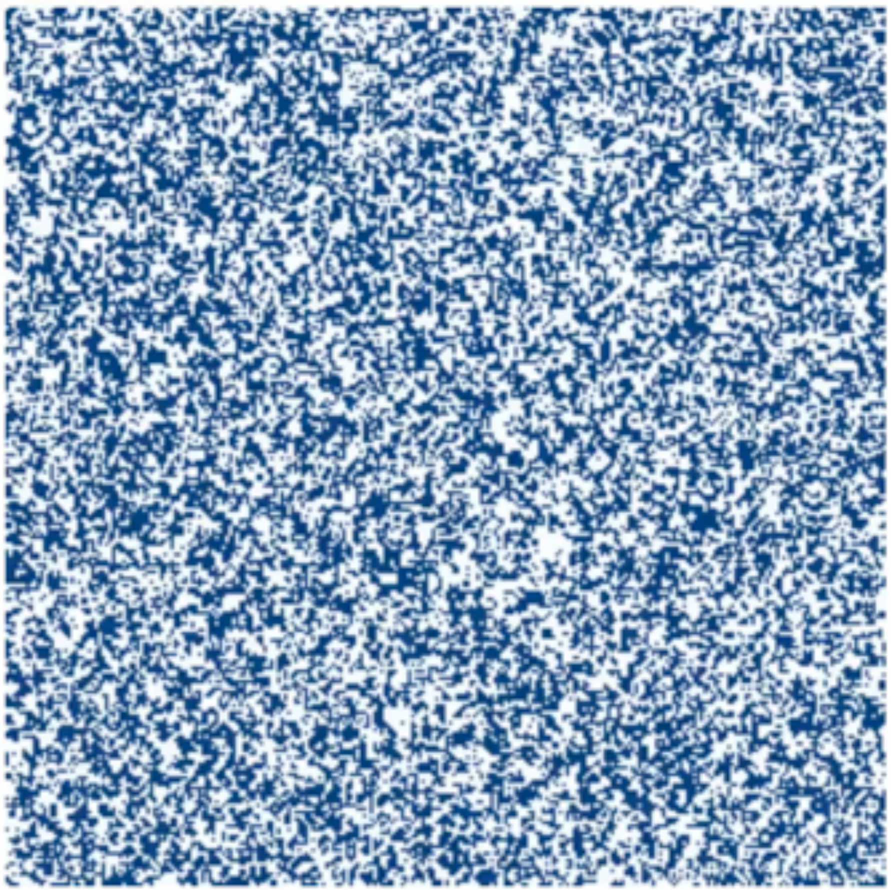


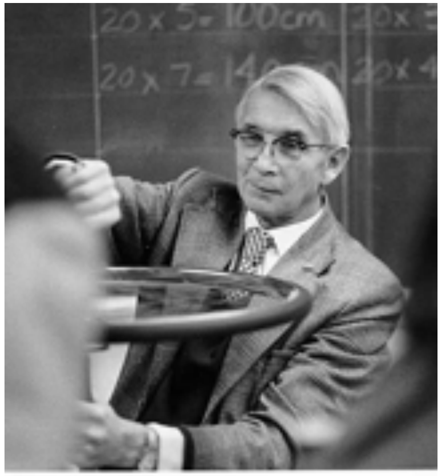
What are the **right images** to feed into the neural network?

classical phases of matter

Finite-temperature transition in the Ising model

$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z$$

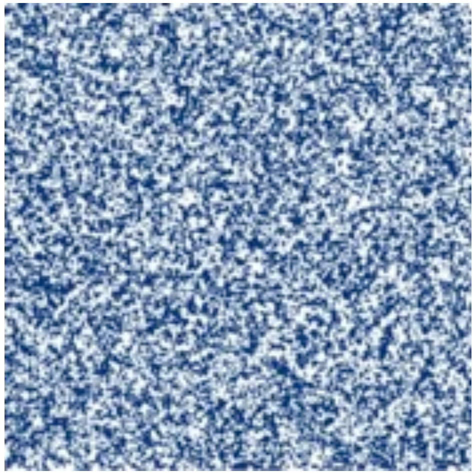




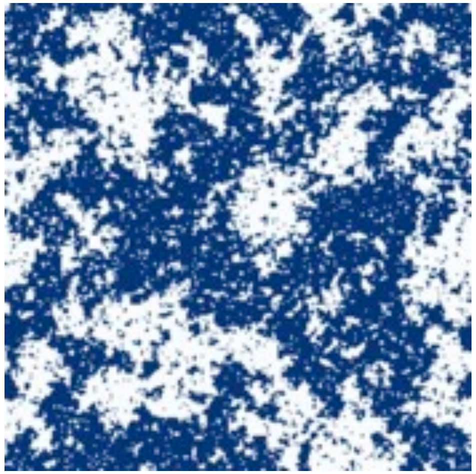
Ernst Ising

classical phases of matter

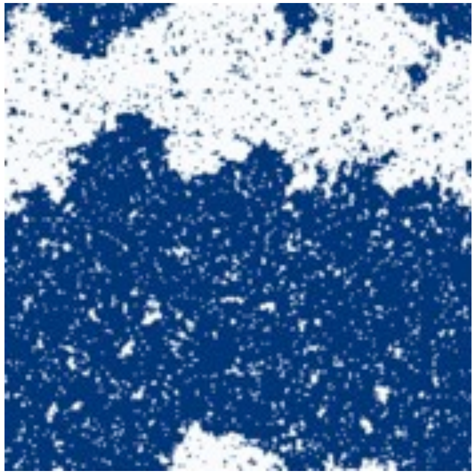
Finite-temperature transition in the Ising model $H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z$



high temperature



“critical” temperature

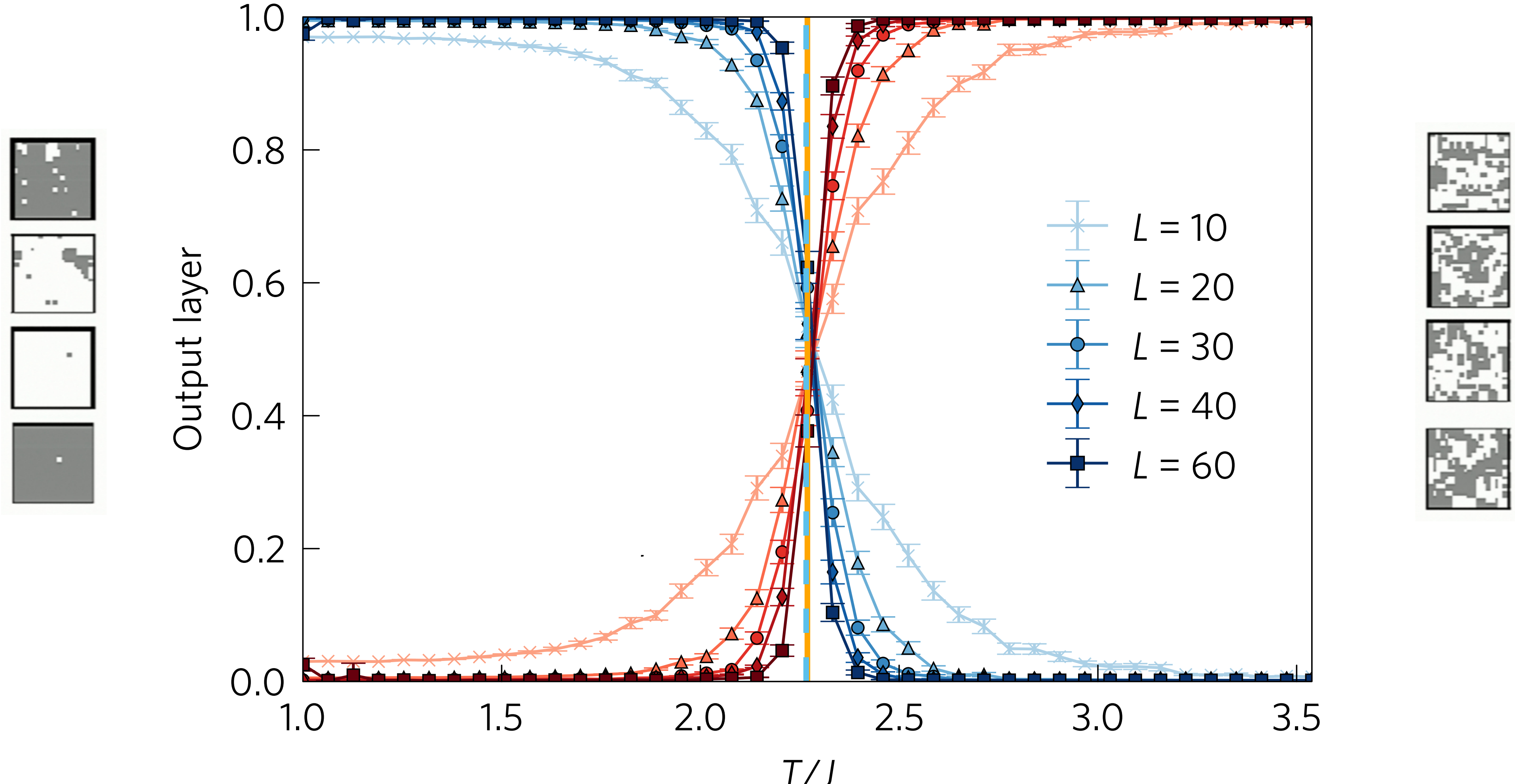


low temperature

classical phases of matter

Carrasquilla and Melko, Nat. Phys. (2017)

Finite-temperature transition in the Ising model $H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z$



classical phases of matter

Carrasquilla and Melko, Nat. Phys. (2017)

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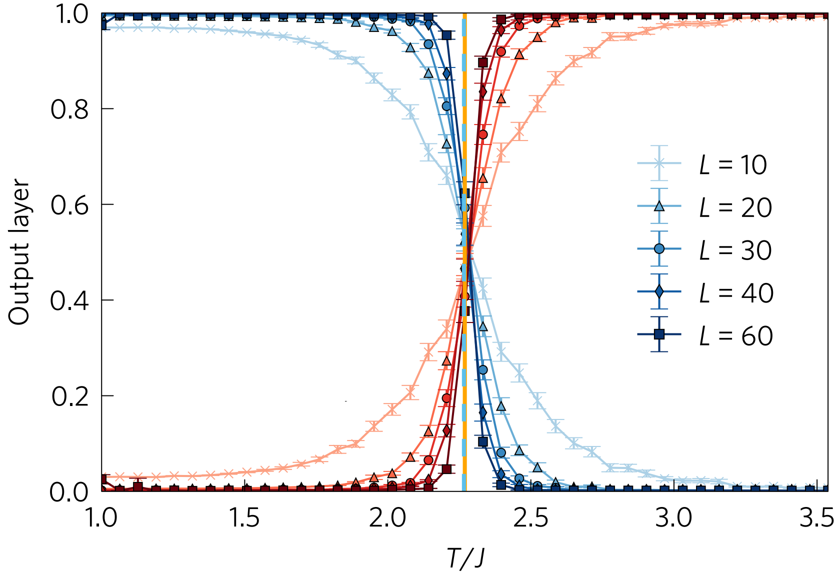

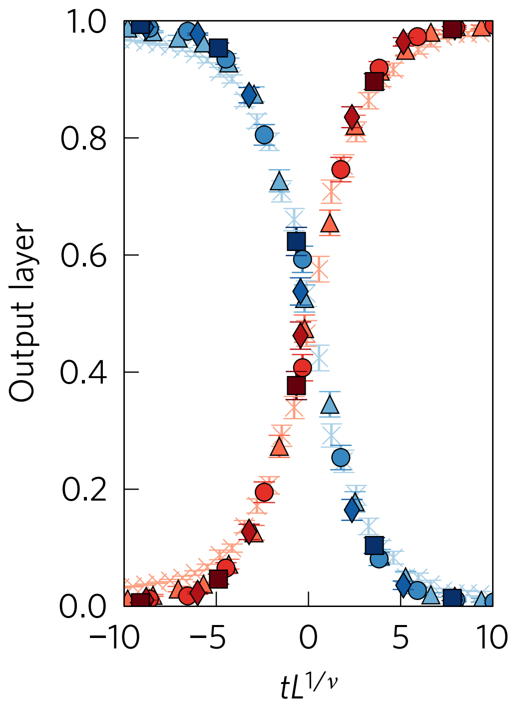

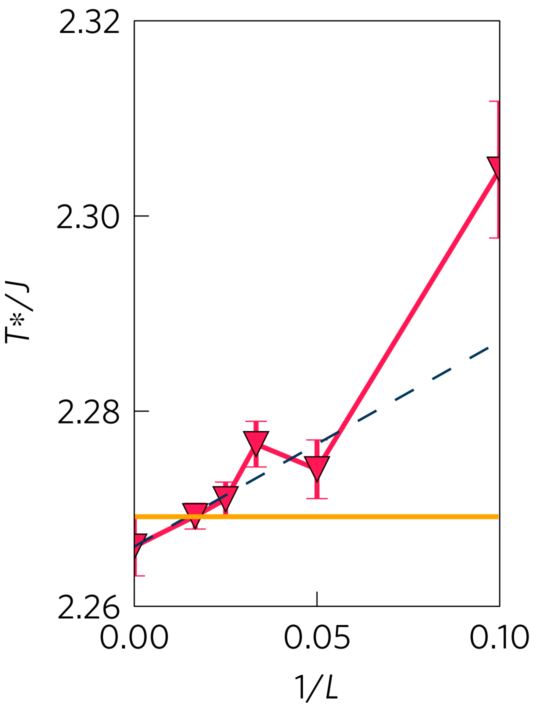

classical phases of matter

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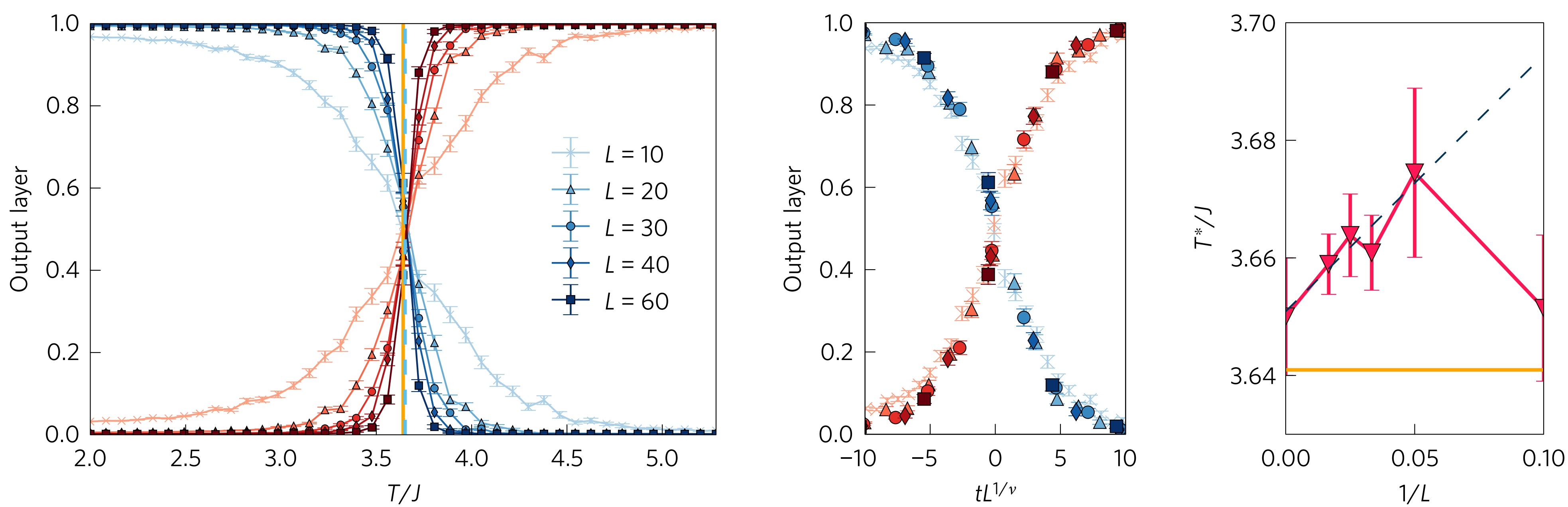
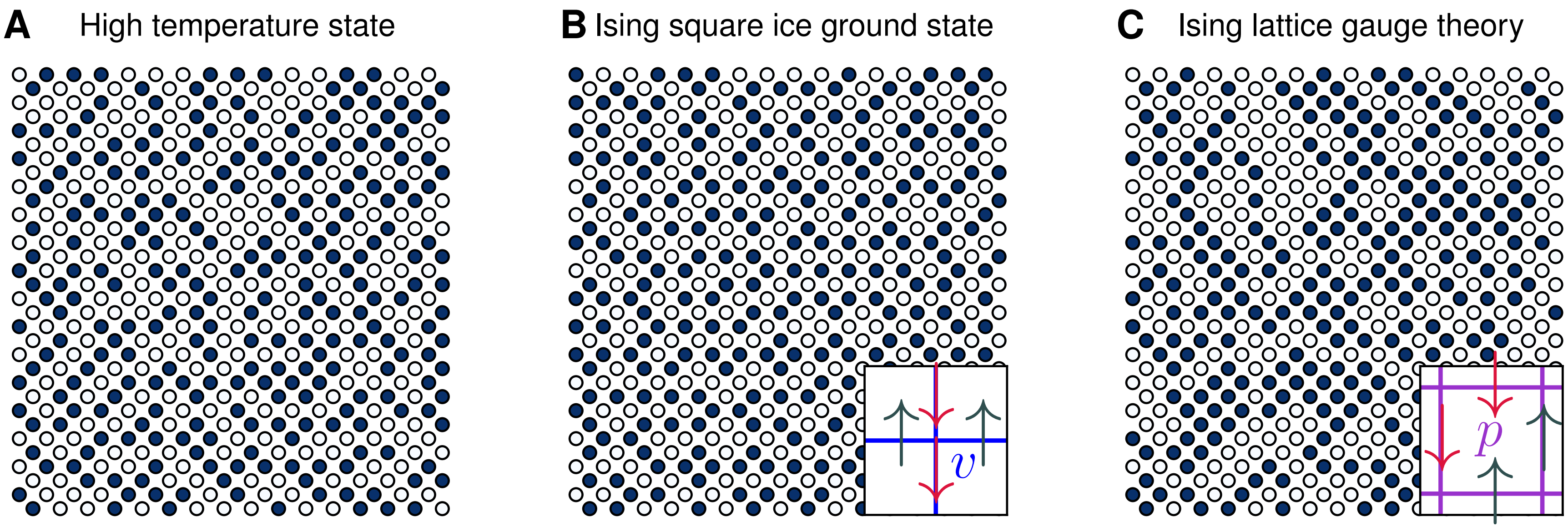


Transfer learning: A neural network trained on the *square* lattice Ising model applied to the *triangular* Ising model correctly identifies its transition.

classical phases of matter

Carrasquilla and Melko, Nat. Phys. (2017)

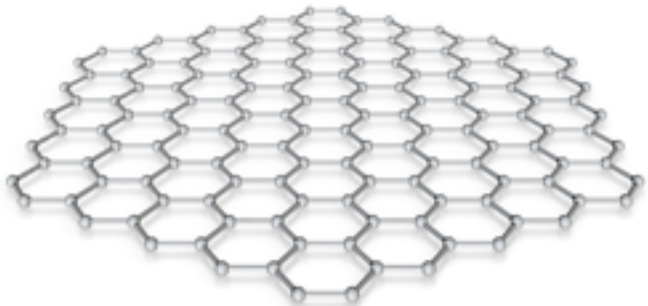


More interestingly, the convolutional neural network can also be trained to distinguish the high-T **paramagnet** from a **Coulomb phase** or **loop gas** ground state, i.e. phases without a local order parameter.

quantum systems

Dirac fermions

Hubbard models on the honeycomb lattice



Spinful fermions

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{\uparrow,i} n_{\downarrow,i}$$

no sign problem

semi-metal | spin density wave → U/t

Gross-Neveu type
fermionic quantum phase transition

Spinless fermions

$$H = -t \sum_{\langle i,j \rangle} \left(c^\dagger_i c_j + c^\dagger_j c_i \right) + V \sum_{\langle i,j \rangle} n_i n_j$$

severe sign problem

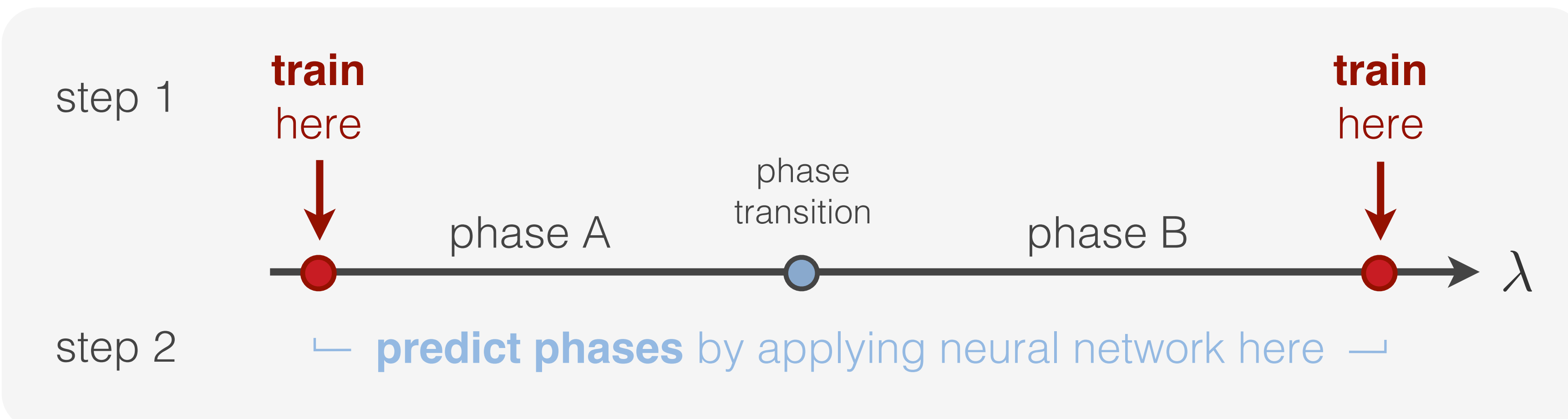
semi-metal | charge density wave → V/t

Supervised learning approach

Supervised learning approach

1) **train** convolutional neural network on representative “images” deep within the two phases

2) apply trained network to “images” sampled elsewhere to **predict phases + transition**



But what are the **right images** to represent a quantum state?

Monte Carlo for fermions

Determinantal (or auxiliary field) quantum Monte Carlo for unbiased studies of strongly interacting fermions

Path integral representation of partition sum

$$\mathrm{Tr}\, e^{-\beta \mathcal{H}} = \mathrm{Tr}\, \left(e^{-\Delta\tau \mathcal{H}}\right)^L \qquad \mathcal{H} = \mathcal{K} + \mathcal{V}$$

Decouple quartic interaction via **Hubbard-Stratonovich** transformation

Now integrate out **free fermions** moving in **background field**

$$\mathcal{Z} = \sum_s \det U(s)$$

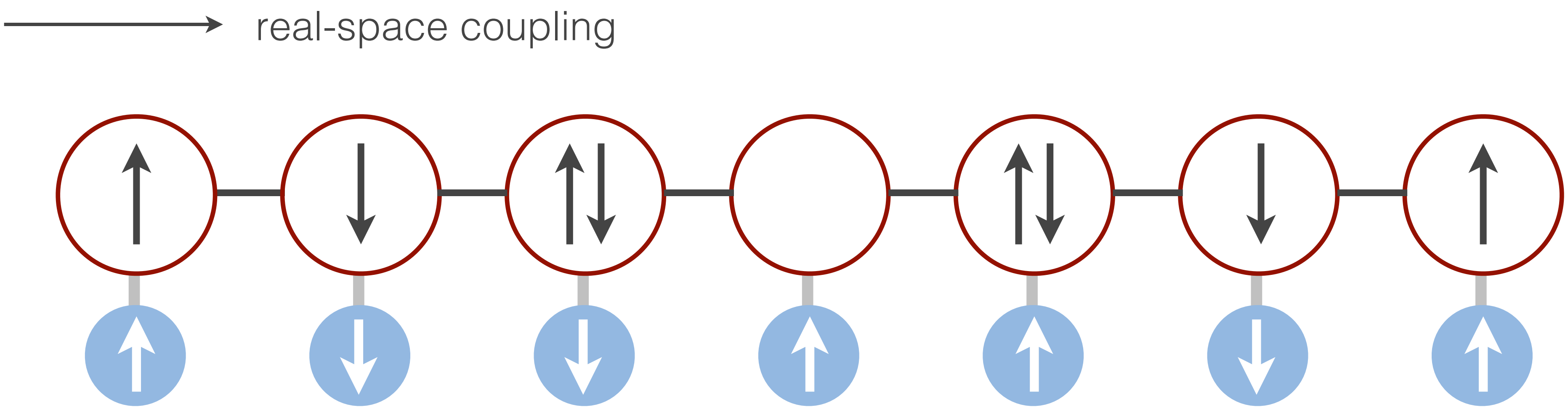
sample **Hubbard-Stratonovich** field

Hubbard-Stratonovich decoupling

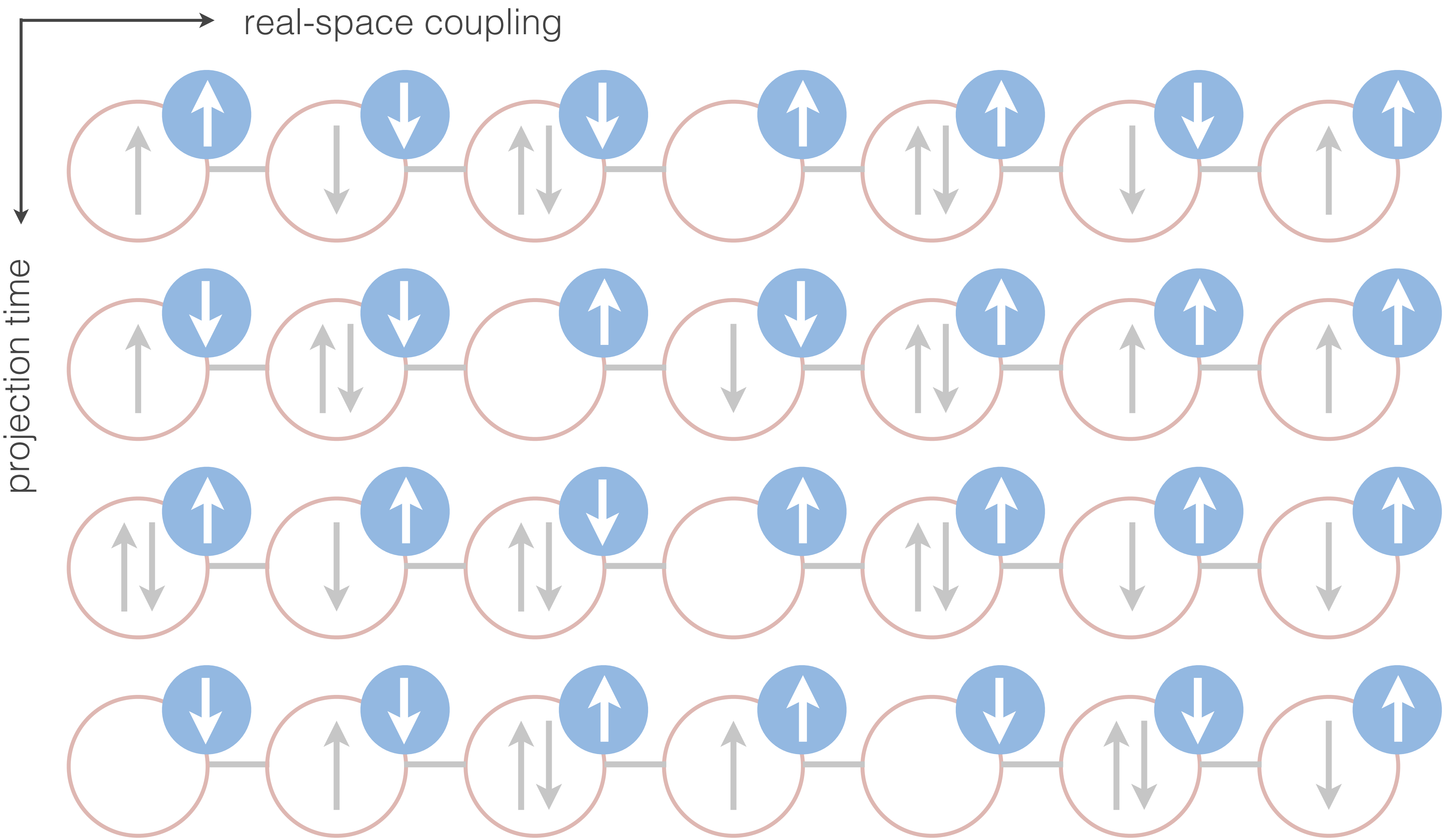
Decoupling quartic interaction via Hubbard-Stratonovich transformation introduces an Ising-type **auxiliary field**

$$V_i = n_i^{\uparrow} n_i^{\downarrow} \longrightarrow V_i(s)$$

Hubbard-Stratonovich decoupling

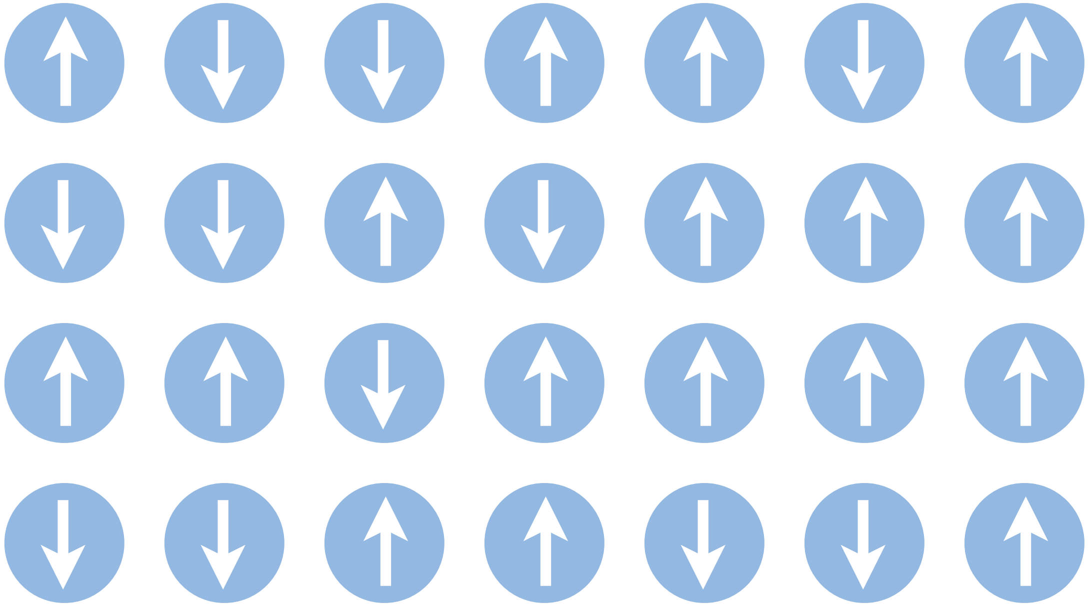


Hubbard-Stratonovich decoupling



Hubbard-Stratonovich decoupling

The auxiliary field has a natural interpretation has **“image”**.



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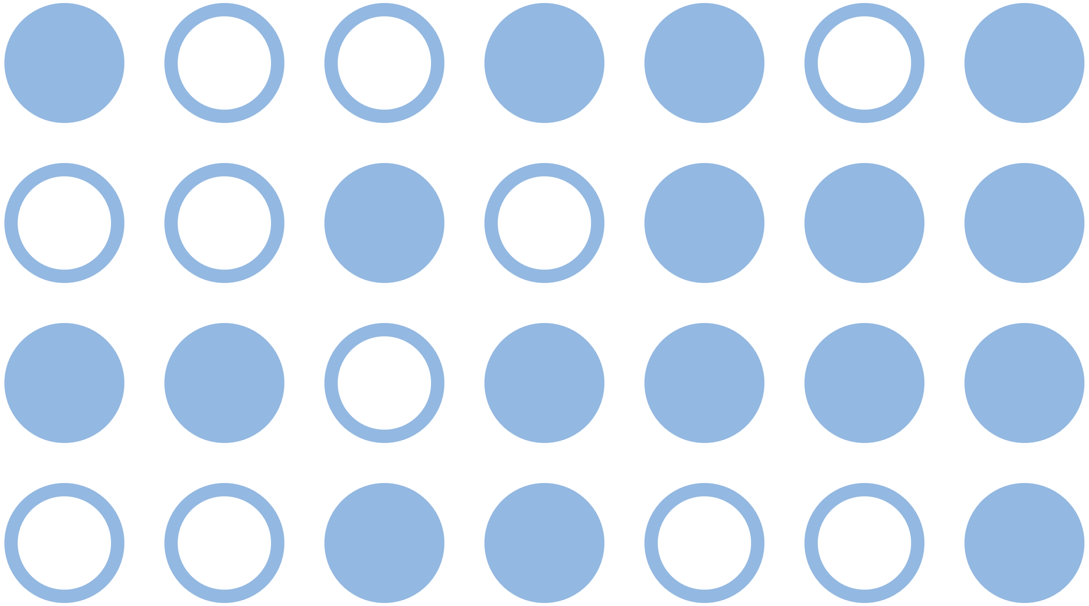


Supervised learning / auxiliary fields

Case 1 – **spinful fermions**

The choice of Hubbard-Stratonovich transformation influences image, i.e. when coupling to ...

magnetization

breaks SU(2)

semi-metal

SDW

charge

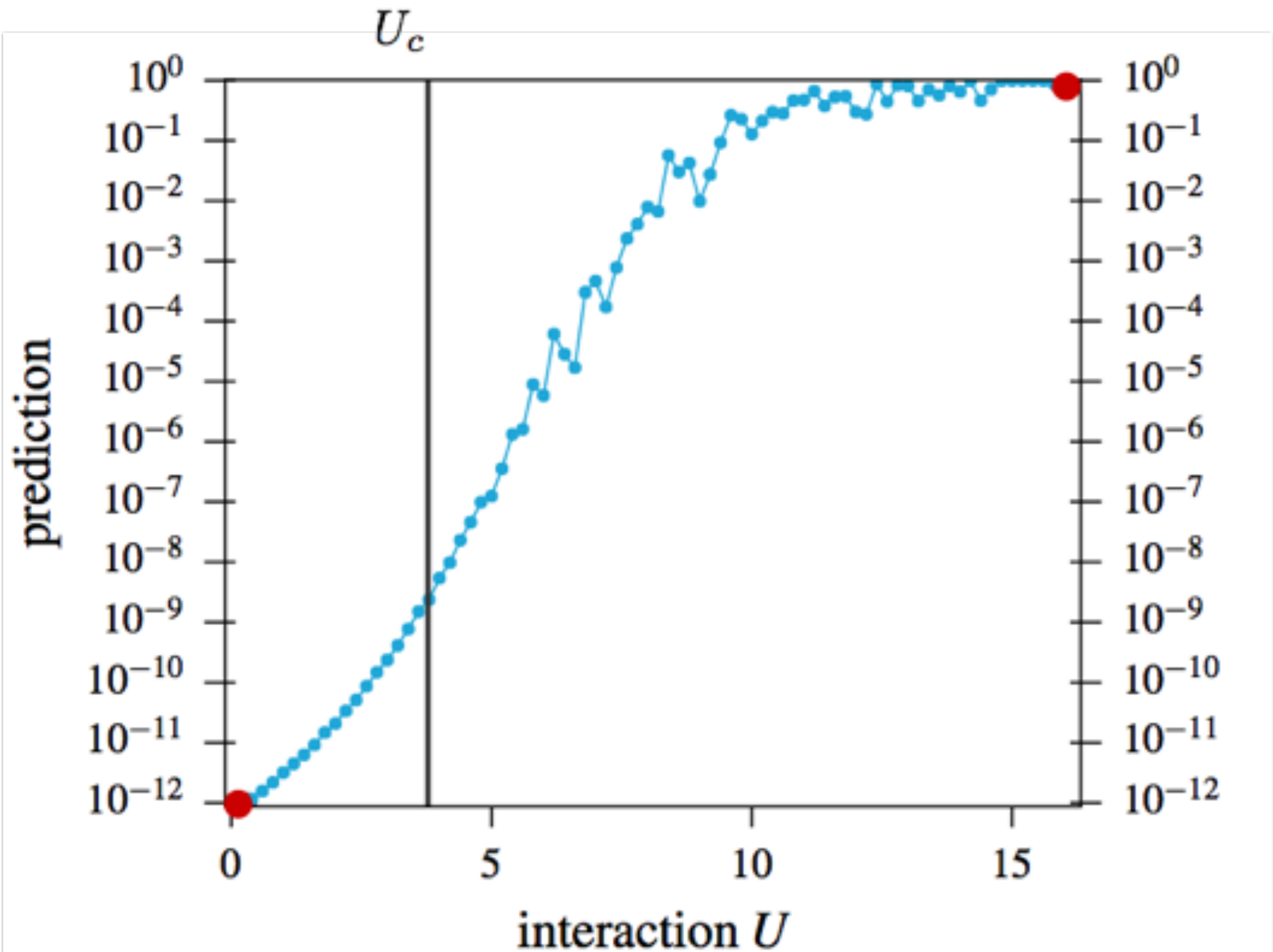
preserves SU(2)

semi-metal

SDW

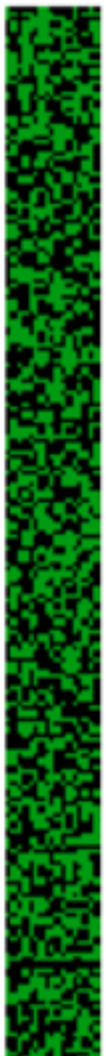
Supervised learning / auxiliary fields

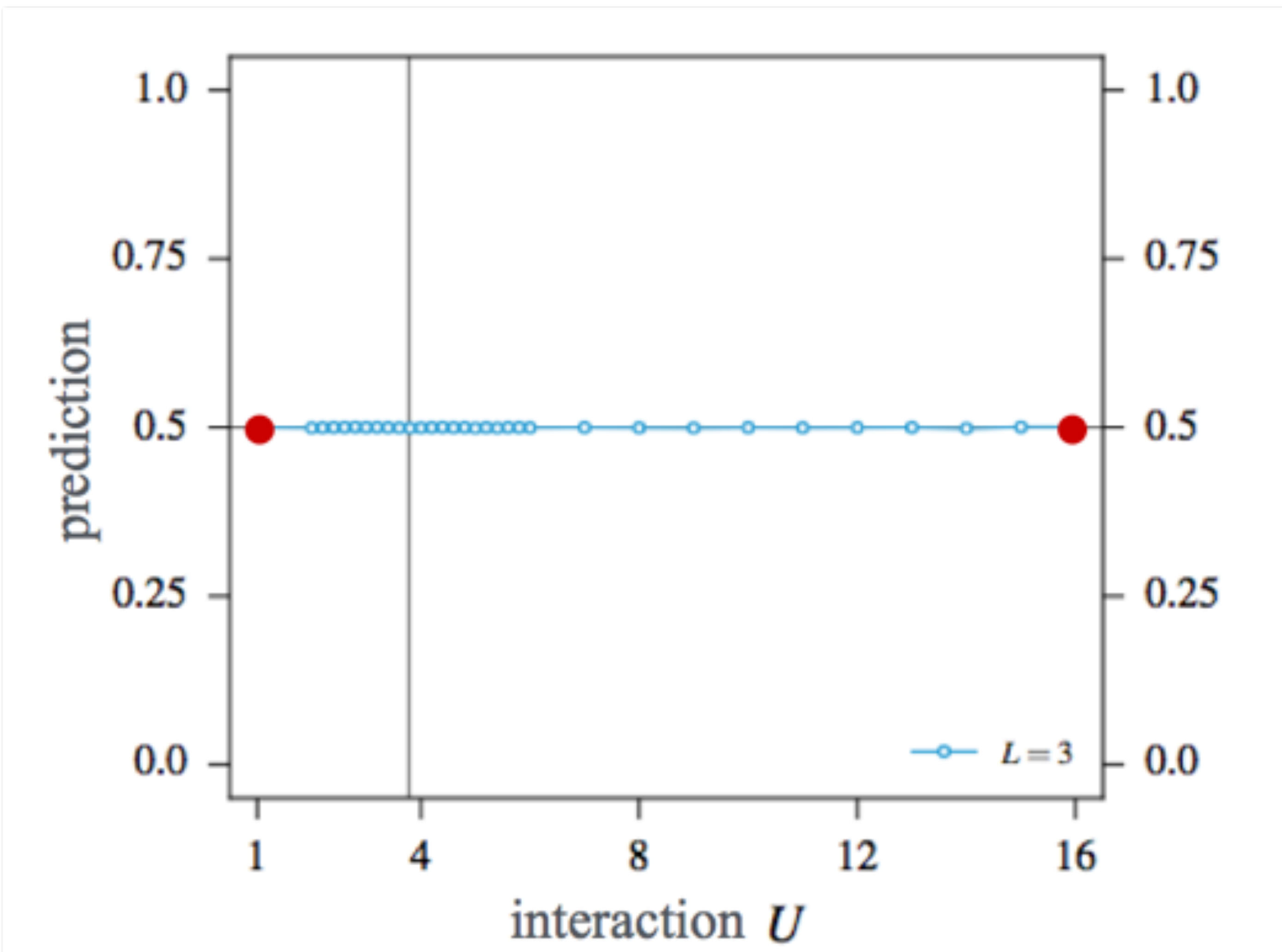
coupling to **magnetization**



Supervised learning / auxiliary fields

coupling to **charge**



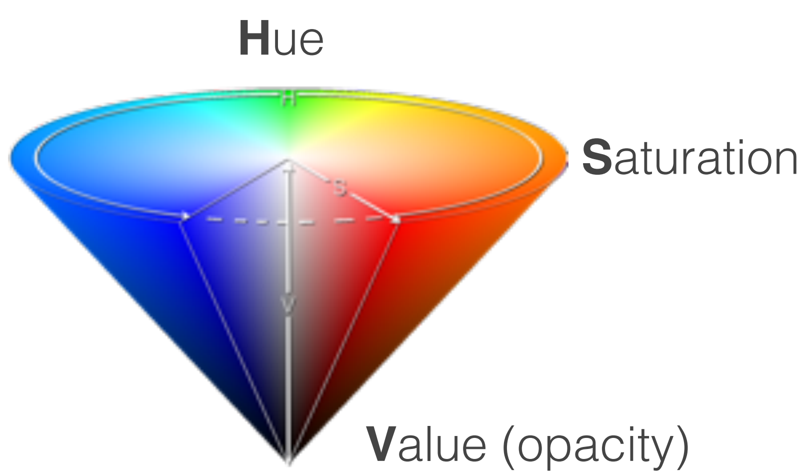


Supervised learning / Green’s functions

Alternative – **Green’s functions** $G(i,j) = \langle c_i c_j^\dagger \rangle$

Green’s functions sampled as **complex valued matrices**.

Convert into color-coded image using HSV color scheme.



Our color mapping

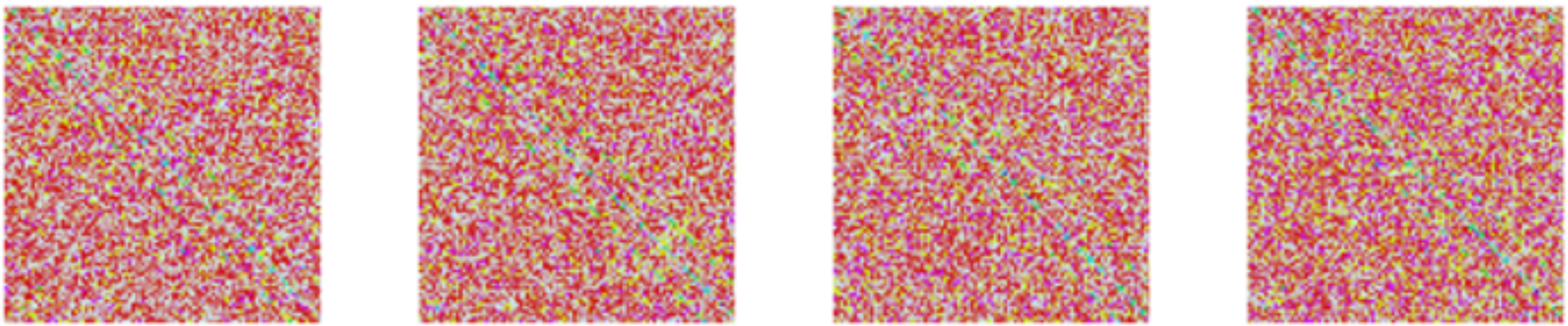
$$c = \underbrace{|c|}_{\text{hue}} \cdot e^{i\phi}$$ saturation

Supervised learning / Green's functions

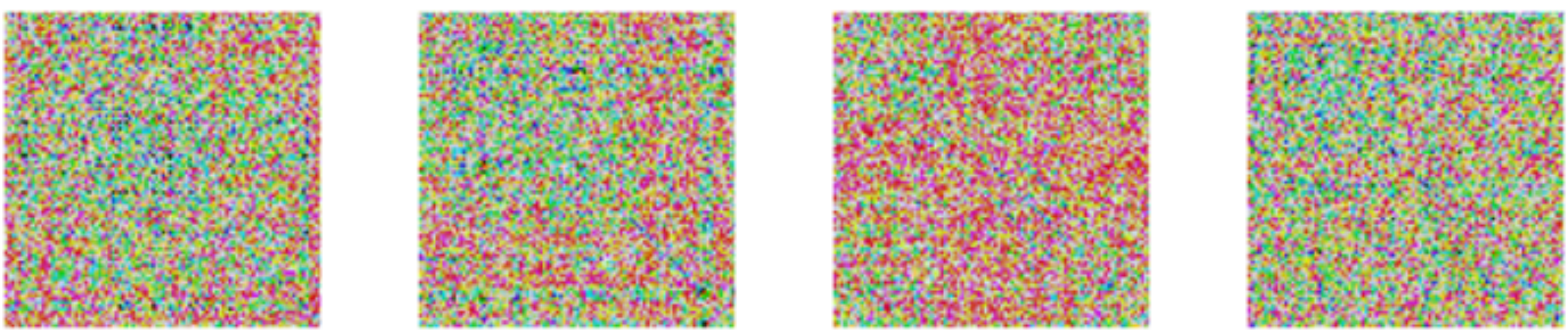
Green's functions for **spinful fermion** model

semi-metal

L = 2x9x9

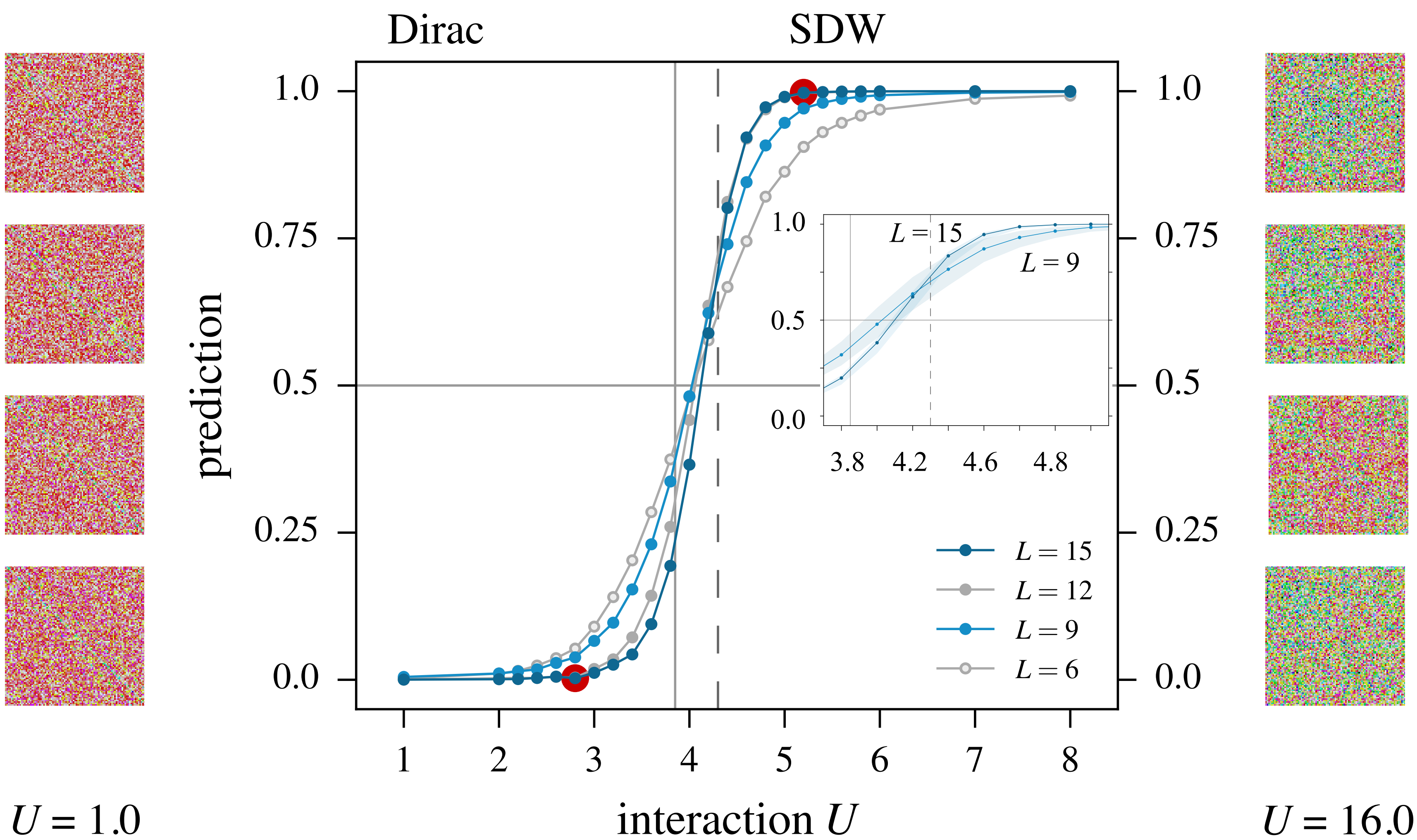


SDW



Spinful fermions

Green's functions are ideal objects/images for machine learning based discrimination of quantum phases.



Some intermediate conclusions

QMC + machine learning approach can be used to distinguish phases of interacting many-fermion systems.

Green's functions are ideal "images" for machine learning.

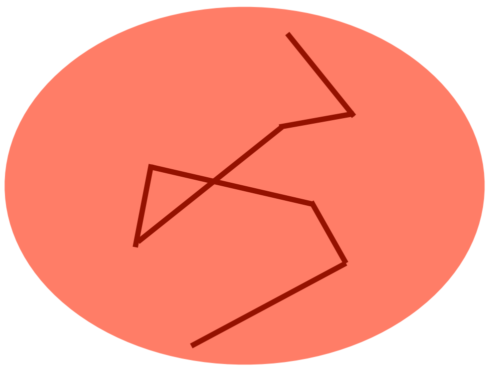
The ensemble of sampled Green's functions contains sufficient information to discriminate fermionic phases.

sign problem

Algorithmic power of Monte Carlo

Sample configurations in **high-dimensional** space

$$c_1 \to c_2 \to \ldots c_i \to c_{i+1} \to \ldots$$



Metropolis (1953): accept new configuration with probability

$$p_{\mathrm{acc}} = \min\left(1, \frac{w(c_j)}{w(c_i)}\right)$$

Simultaneously measured observables converge in **polynomial time**.

Tremendous impact across many different fields.

In hard condensed matter

- percolation
- phase transitions
- quantum magnetism
- ultracold bosons

Quantum Monte Carlo

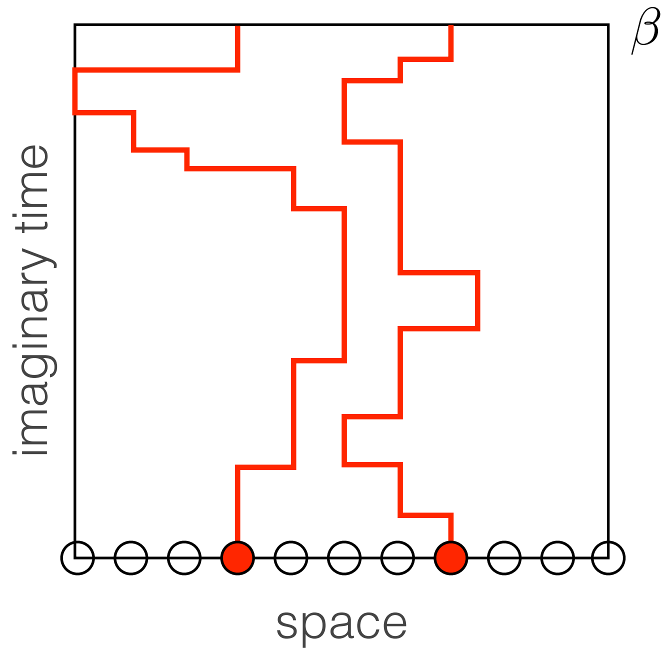
classical Monte Carlo $$\langle \mathcal{O} \rangle = \frac{\sum_{\mathcal{C}} \mathcal{O}(\mathcal{C})\, e^{-\beta E(\mathcal{C})}}{\sum_{\mathcal{C}} e^{-\beta E(\mathcal{C})}}$$

quantum Monte Carlo $$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}\, \mathcal{O} e^{-\beta \mathcal{H}}}{\mathrm{Tr}\, e^{-\beta \mathcal{H}}}$$

Map quantum to classical system $$Z = \mathrm{Tr}\, e^{-\beta \mathcal{H}} = \sum_{\mathcal{C}} p(\mathcal{C})$$

Map to “**world lines**” of the trajectories of the particles

Monte Carlo sampling of these world lines



The sign problem

Expectation value for observables

$$\langle \mathcal{O} \rangle = \frac{\sum \mathcal{O}(C) p(\mathcal{C})}{\sum p(\mathcal{C})}$$

when we **ignore the sign** of the configuration weights.

... but the **average sign decreases exponentially**

$$\langle \sigma \rangle_{\text{abs}} = \frac{\sum \sigma(C) |p(\mathcal{C})|}{\sum |p(\mathcal{C})|} = \frac{Z}{Z_{\text{abs}}} = \exp\left(-\beta N \Delta f\right)$$

... resulting in an **exponentially slow convergence** of the statistical error

$$\frac{\Delta\sigma}{\langle\sigma\rangle} = \frac{\sqrt{\langle\sigma^2\rangle - \langle\sigma\rangle^2}}{\sqrt{M}\langle\sigma\rangle} \approx \frac{e^{\beta N \Delta f}}{\sqrt{M}}$$

Fundamental limit for quantum Monte Carlo simulations of

- fermions
- many-electron systems
- frustrated quantum magnetism, spin liquids

Is there a way out?

The sign problem is **basis dependent**

energy eigenbasis $\longleftrightarrow$ simulation basis

exponentially hard

Successful **basis changes**

meron cluster — Wiese et al., PRL (1995)

fermion bag — Chandrasekharan, PRD (2009)

Majorana fermion basis — Yao et al., PRB (2015)

no general solution — Troyer and Wiese, PRL (2005) — the sign problem is **NP-hard**

Change of **perspective**

effective, sign-problem free actions — Berg, Metlitski, and Sachdev, Science (2012)

entanglement entropies — Broecker and Trebst, PRB (2016)

sign problem
+ machine learning

arXiv:1608.07848

Can we bypass the sign problem?

QMC sampling + **statistical analysis**

$$\langle \mathcal{O} \rangle = \frac{\sum \mathcal{O}(C) p(\mathcal{C})}{\sum p(\mathcal{C})} = \frac{\sum \mathcal{O}(C) \sigma(\mathcal{C}) |p(\mathcal{C})|}{\sum \sigma(\mathcal{C}) |p(\mathcal{C})|} = \frac{\langle \mathcal{O} \cdot \sigma \rangle_{\mathrm{abs}}}{\langle \sigma \rangle_{\mathrm{abs}}}$$

QMC sampling + **machine learning**

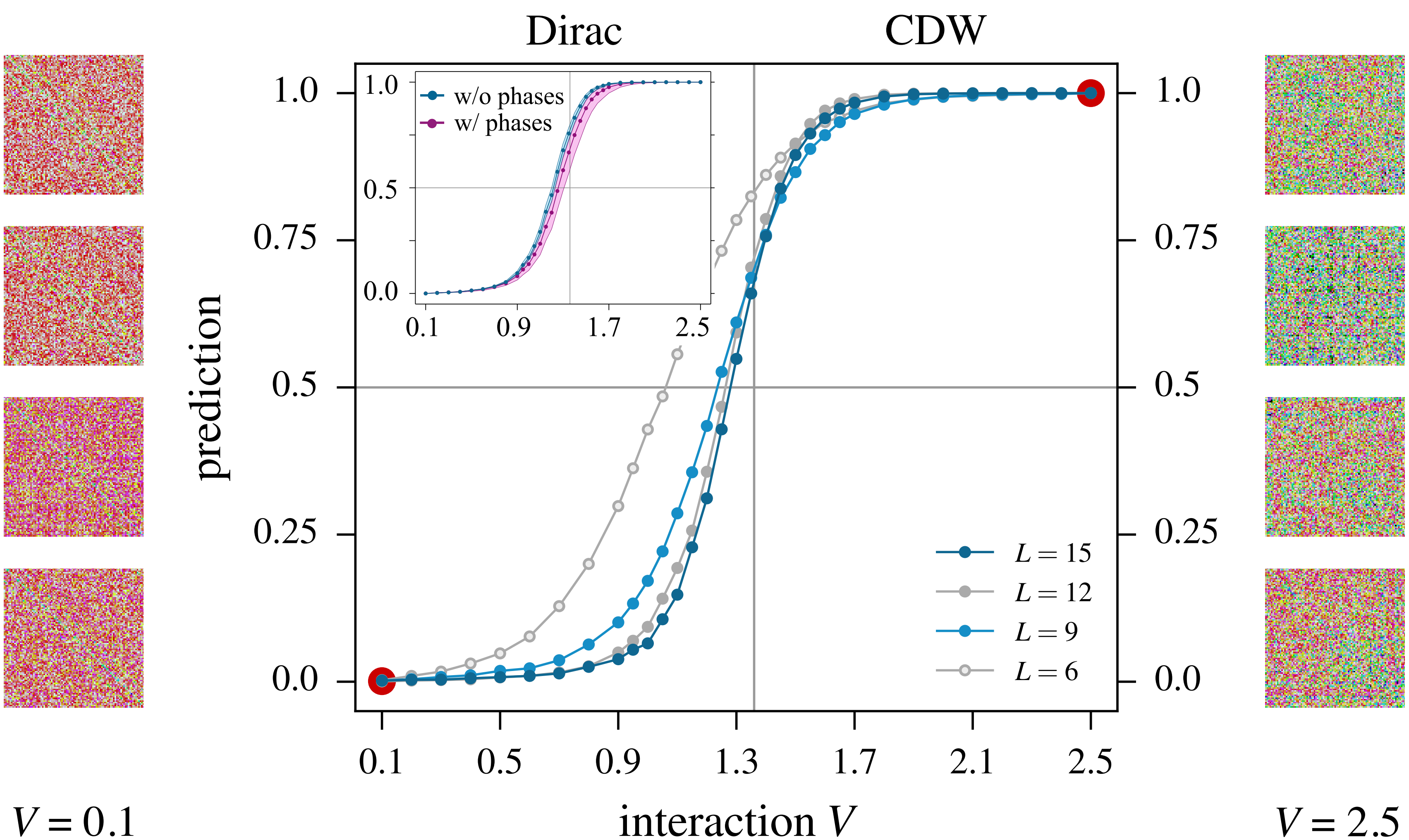
Assume there exists a "state function"

$$\langle \mathcal{F} \rangle_{\mathrm{abs}} = \frac{\sum \mathcal{F}(C) |p(\mathcal{C})|}{\sum |p(\mathcal{C})}$$

that is 0 deep in phase A and 1 deep in phase B.

Spinless fermions

QMC + machine learning approach gives useful results even for systems with a severe sign problem.



unsupervised learning

Peter Broecker, Fakher Assaad, and ST, in preparation
related ideas in Evert van Nieuwenburg, Ye-Hua Liu, and Sebastian Huber, Nature Physics (2017)

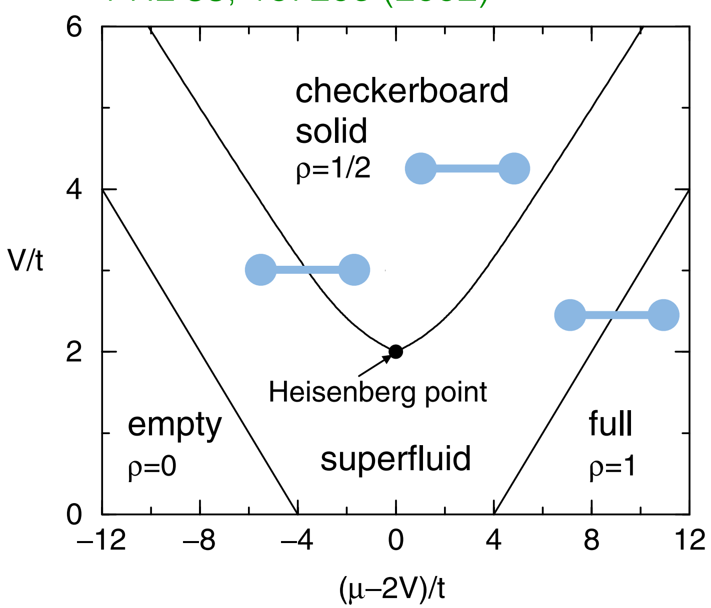
Unsupervised learning

Employ ability to “blindly” distinguish phases to map out an entire phase diagram with no hitherto knowledge about the phases.

Example: hardcore bosons / XXZ model on a square lattice

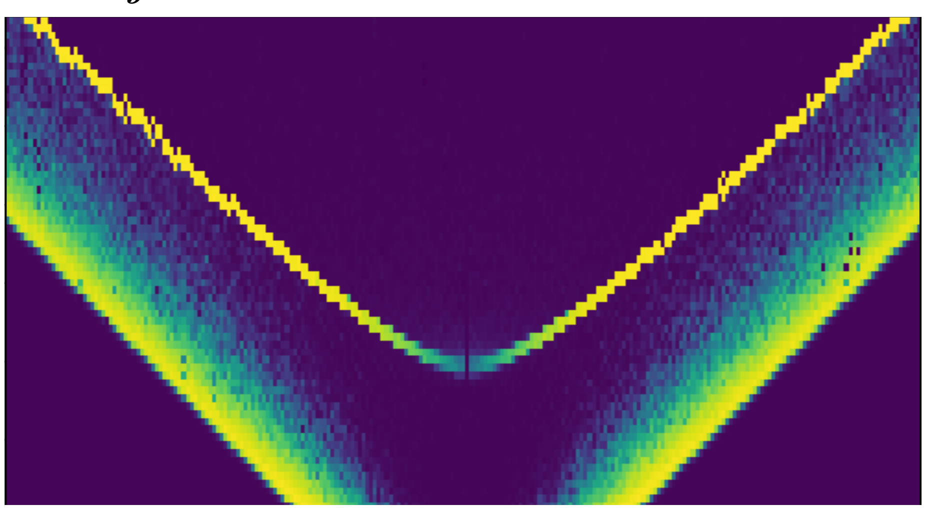
$$H = -\sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + \Delta \sum_{\langle i,j \rangle} S_i^z S_j^z + h \sum_i S_i^z$$

PRL **88**, 167208 (2002)



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

preliminary results



-12 h 12

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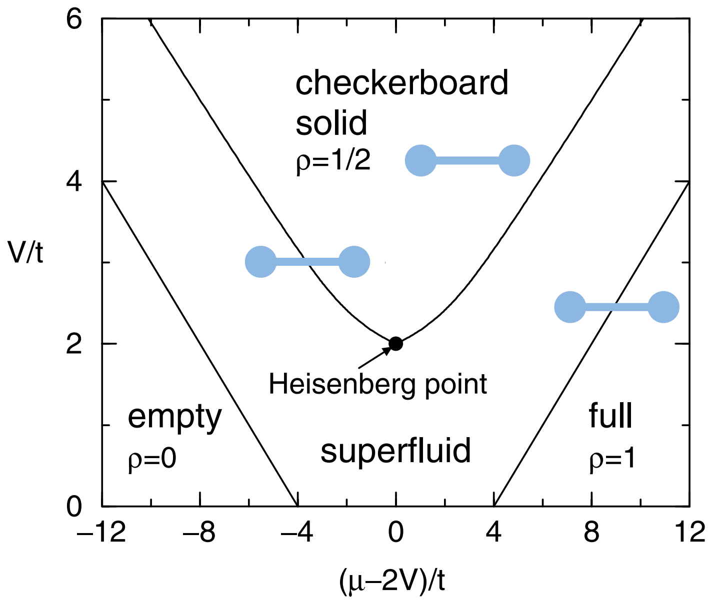
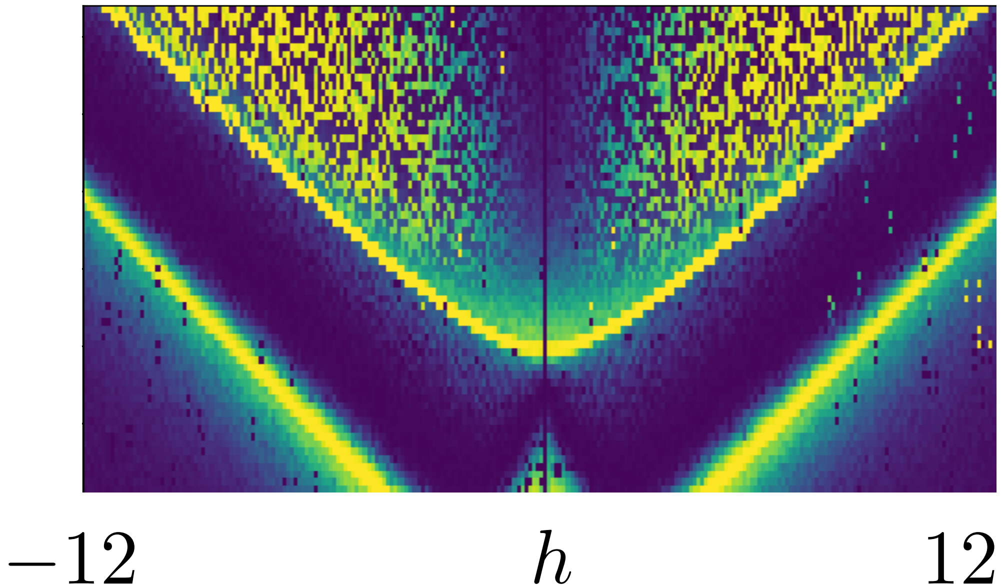


$\langle S_i^+ S_j^- \rangle + \langle S_i^- S_j^+ \rangle$ preliminary results

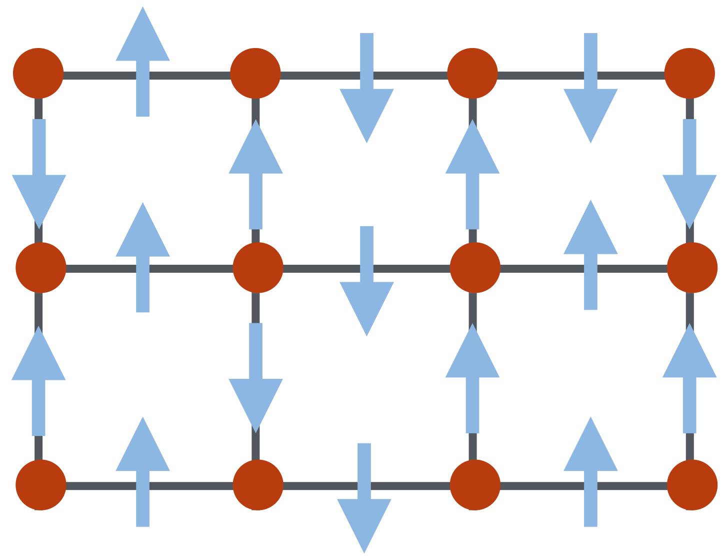


Topological order

Assaad and Grover, PRX (2016)
Gazit, Randeria & Vishwanath, Nature Physics (2017)

Toy model for topological order in a fermionic system:
fermions coupled to (quantum) Z_2 (Ising) spins on bonds

$$H = \sum_{\langle i,j \rangle} Z_{\langle i,j \rangle} \left(\sum_{\alpha=1}^{N} c_{i,\alpha}^{\dagger} c_{j,\alpha} + h.c. \right) + Nh \sum_{\langle ij \rangle} X_{\langle i,j \rangle}$$



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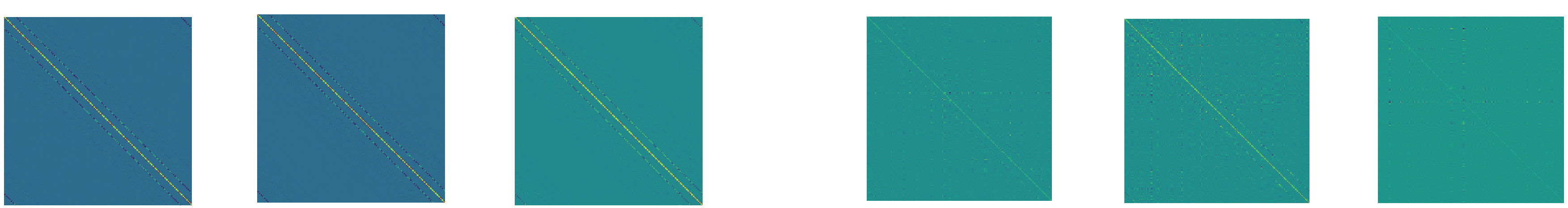

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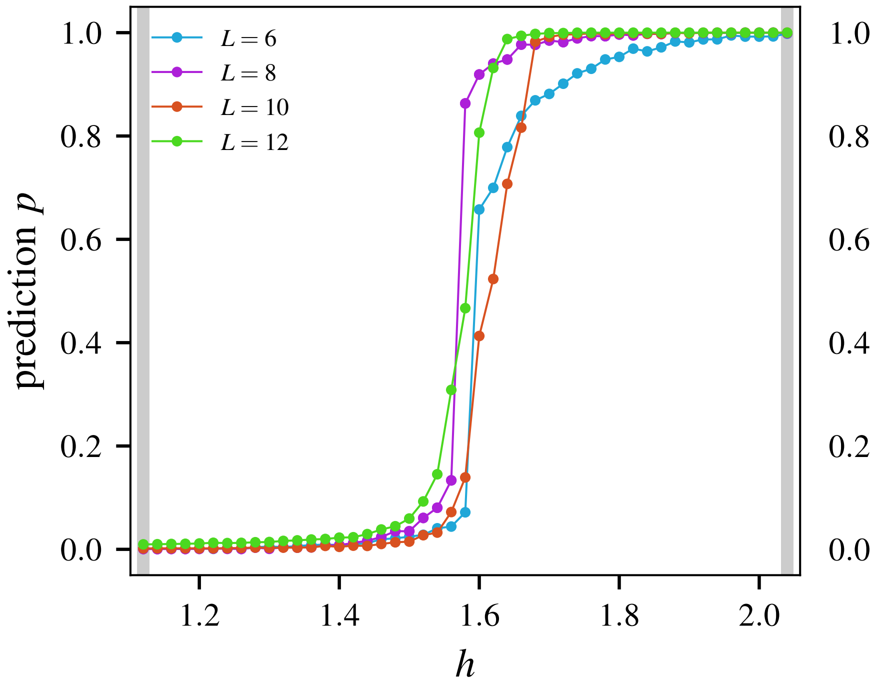
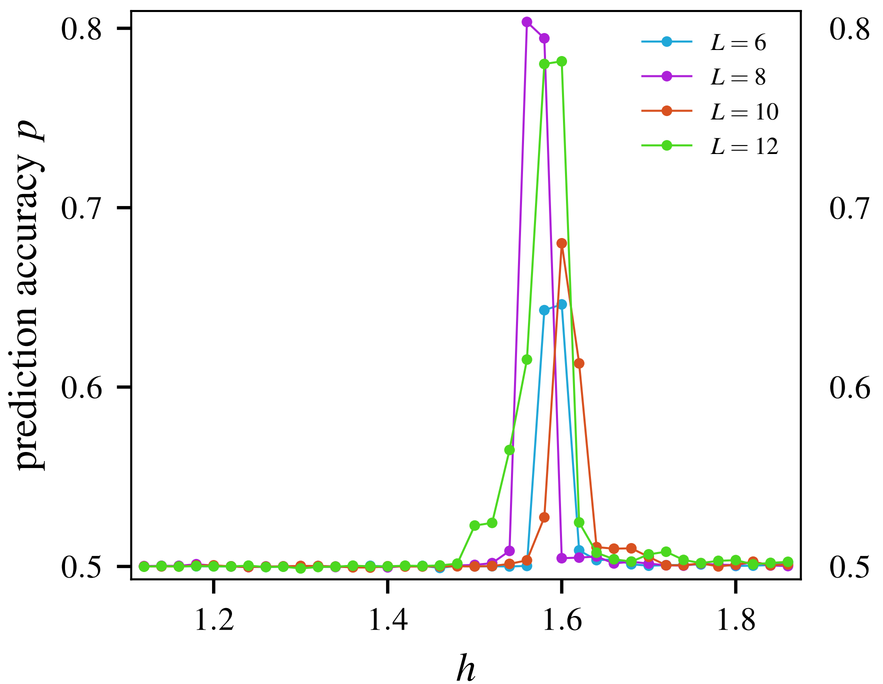
supervised approach



unsupervised approach

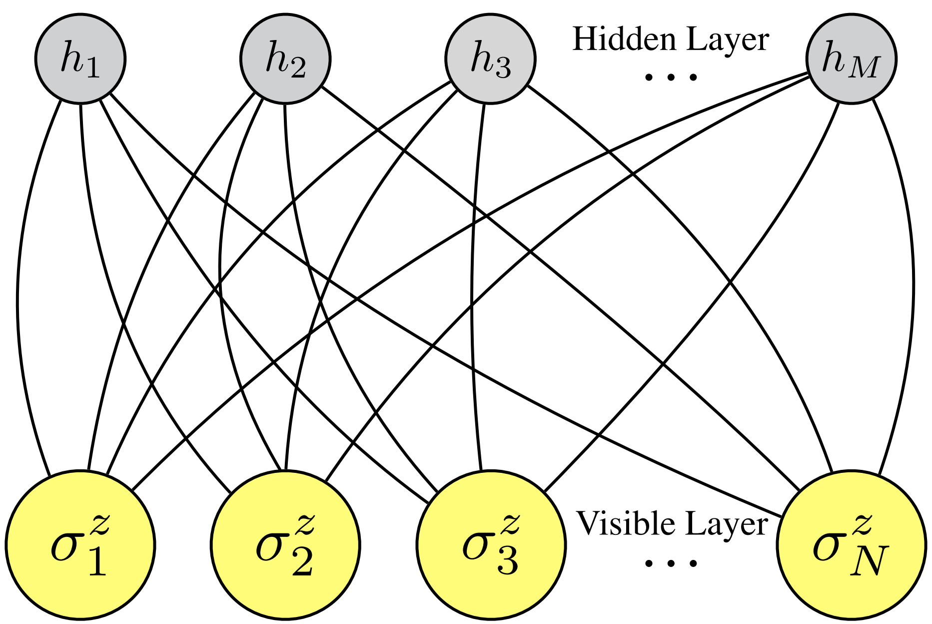


quantum state tomography

Giuseppe Carleo and Matthias Troyer, Science 355, 602 (2017)

quantum state tomography

Carleo and Troyer, Science (2017)



M hidden neurons
(auxiliary spin variable)

accuracy can be tuned
by adjusting α=*M/N*

restricted Boltzmann machine

$$\Psi(\sigma_1^z, \sigma_2^z, \ldots \sigma_N^z; \mathbf{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

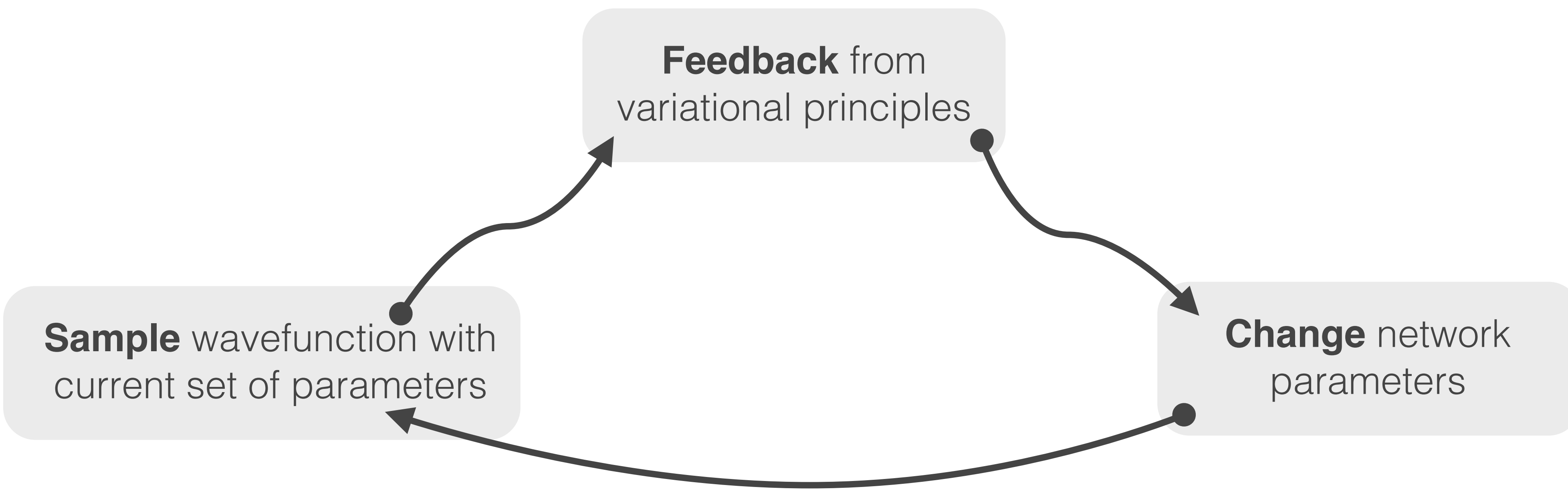
Variational Parameters

quantum state tomography

Carleo and Troyer, Science (2017)

$$\Psi(\sigma_1^z, \sigma_2^z, \ldots \sigma_N^z; \mathbf{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

Variational Parameters

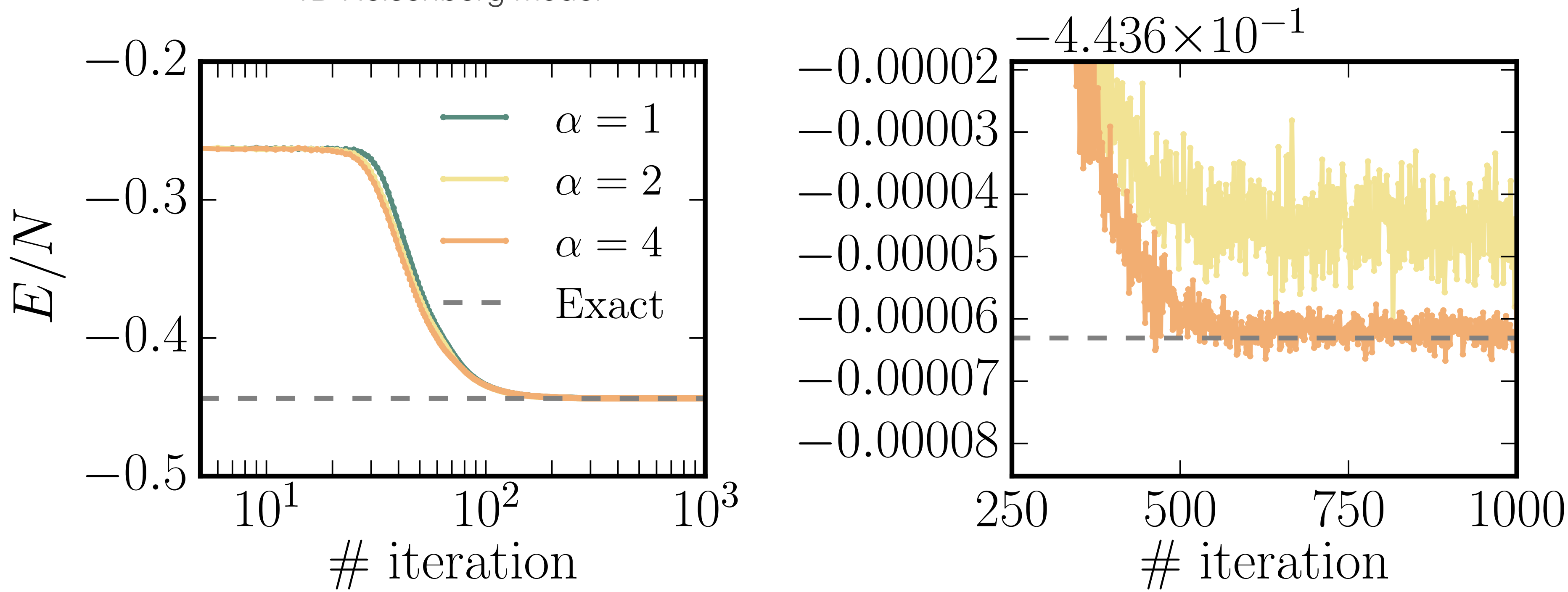


quantum state tomography

Carleo and Troyer, Science (2017)

Variational energies.

1D Heisenberg model



quantum state tomography

Carleo and Troyer, Science (2017)

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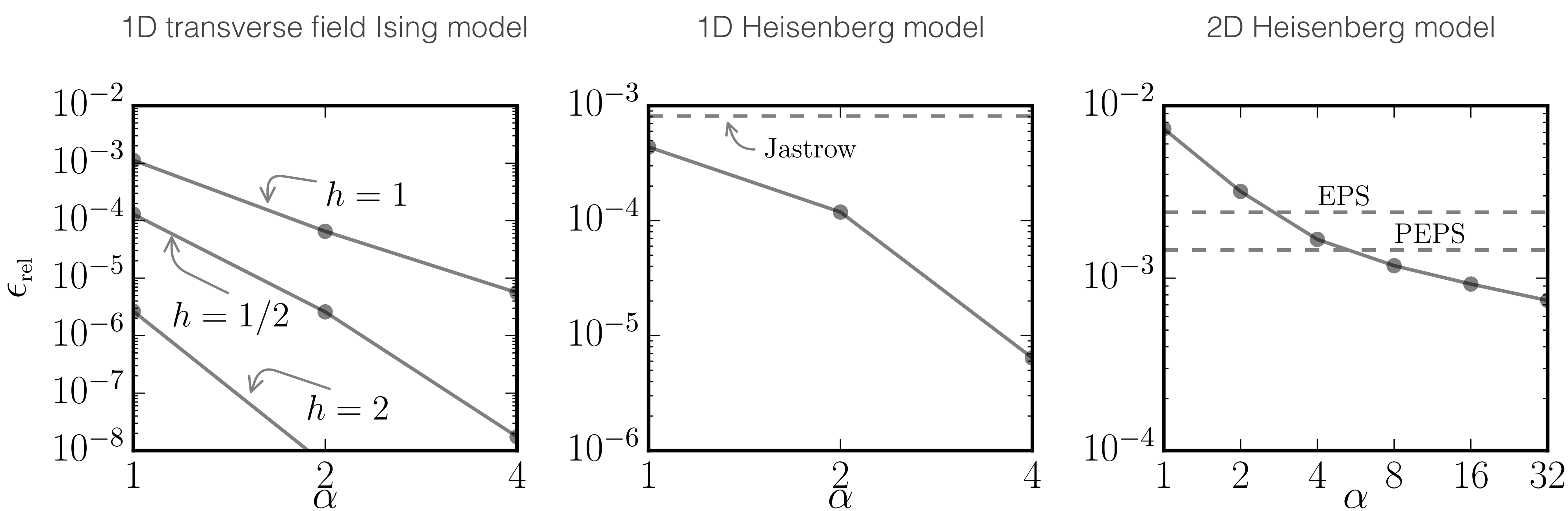

very high precision, limited only by stochastic sampling

compact representation
~10^2 less parameters than corresponding MPS in 1D

improvements over best PEPS results

summary

Summary

QMC + machine learning approaches can be used to distinguish phases of interacting quantum many-body systems (and opens opportunities to overcome the sign problem).

There are a number of interesting analytical connections between neural networks and matrix product states as wells as the renormalization group.

This is just the beginning. Probably, we will see, in the coming years, a similarly productive interplay between machine learning and quantum statistical physics as we have seen with quantum information.

arXiv:1608.07848

Thanks!

@SimonTrebst