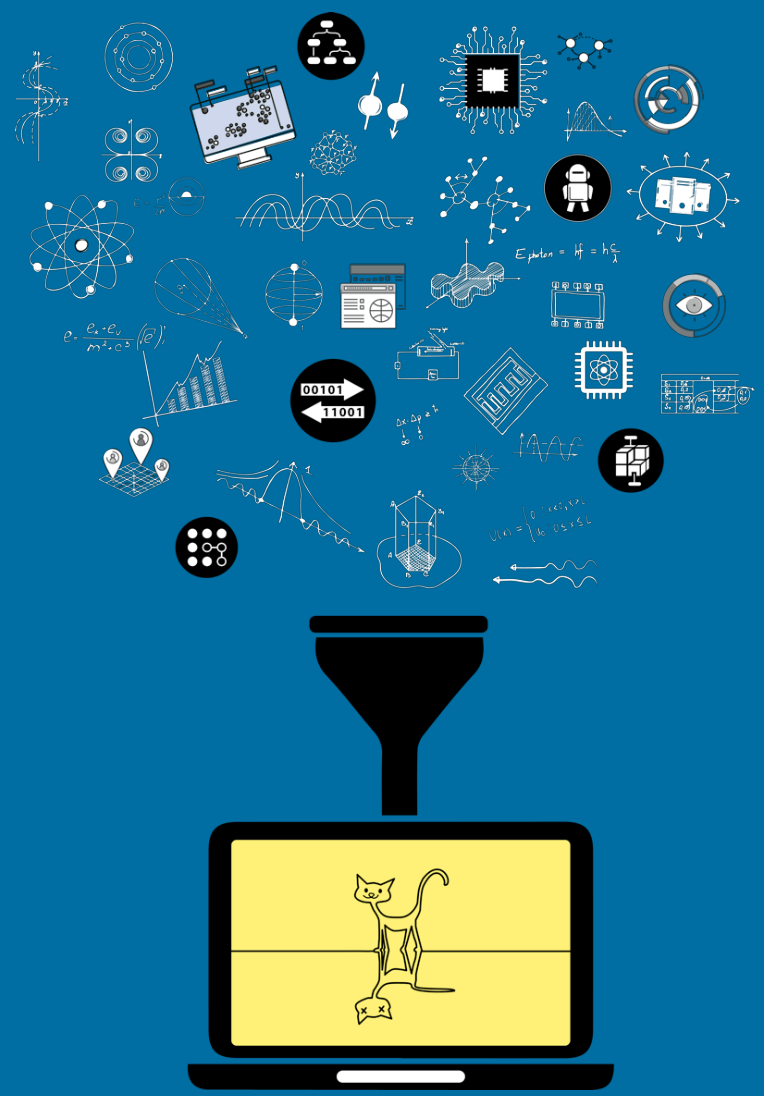
Decoding the many-fermion problem with neural networks

KITP Santa Barbara
March 2019

Simon Trebst
University of Cologne



CRC183
ENTANGLED STATES OF MATTER

collaborators

Peter Broecker

Juan Carrasquilla
Roger Melko

Fakher Assaad

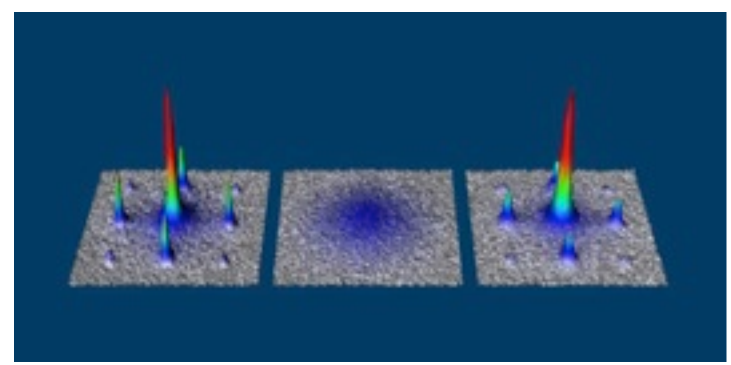
Carsten Bauer
Yi Zhang
Eun-Ah Kim

prelude

Quantum matter

water ice

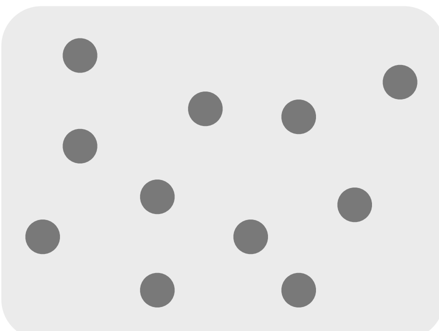
superconductor



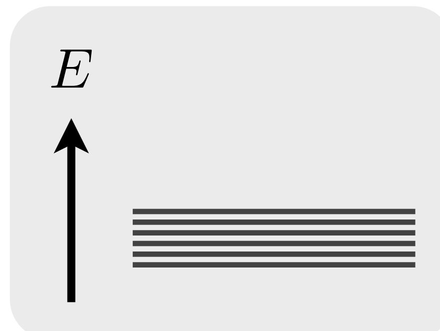
Bose-Einstein condensate

When do interesting things happen?

Some of the most intriguing phenomena in condensed matter physics arise from the splitting of ‘accidental’ degeneracies.



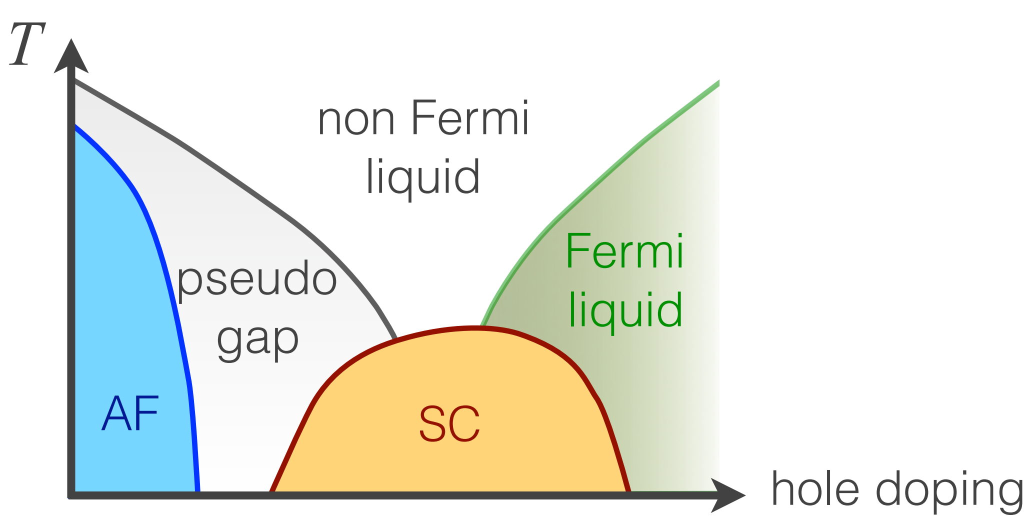
interacting
many-body system



‘accidental’
degeneracy

residual effects
select ground state

phase diagram of
cuprate superconductors



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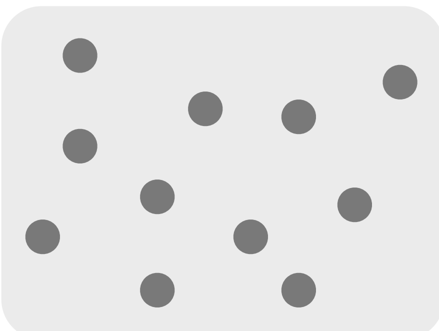

interacting
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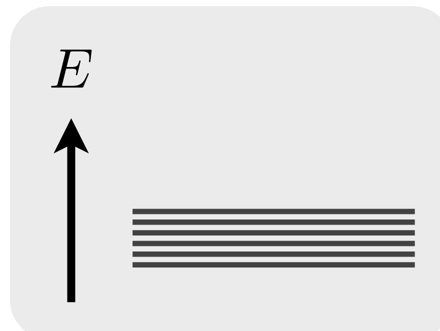


‘accidental’
degeneracy

residual effects
select ground state

But they are also notoriously difficult to handle, due to

- multiple energy scales
- complex energy landscapes / slow equilibration
- macroscopic entanglement
- strong coupling

quantum many-body simulations

statistical physics

The **quantum many-body problem**:
What is the ground state of a macroscopic number of interacting bosons, spins or fermions?

A continuous **stream of computational and conceptual advances** has been directed towards attacking this problem:

- quantum Monte Carlo (non-local updates)
- density matrix renormalization group
- entanglement perspective
- tensor network states

statistical physics + machine learning

The **quantum many-body problem**:
What is the ground state of a macroscopic number of interacting bosons, spins or fermions?

Machine learning approaches:

- dimensional reduction
- feature extraction

A **perfect match** for the goal of identifying essential characteristics of a quantum many- body system, but often hidden in

- exponential complexity of its many-body wavefunction
- abundance of potentially revealing correlation functions

machine learning

But there is also an **abundance of machine learning** approaches

- supervised learning
- unsupervised learning
- reinforcement learning

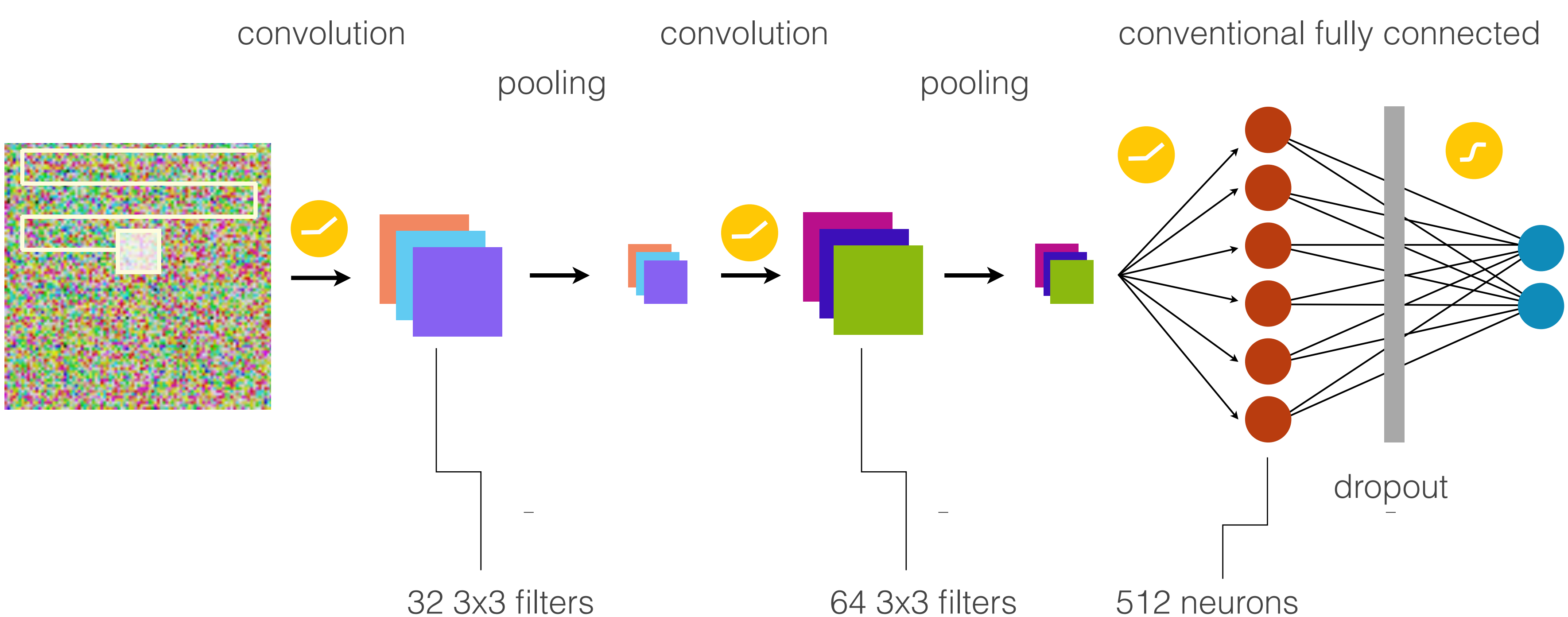
that are oftentimes built around **artificial neural networks**

- restricted Boltzmann machines (RBMs)
- generative adversarial network (GANs)
- convolutional neural networks (CNNs)

today's menu

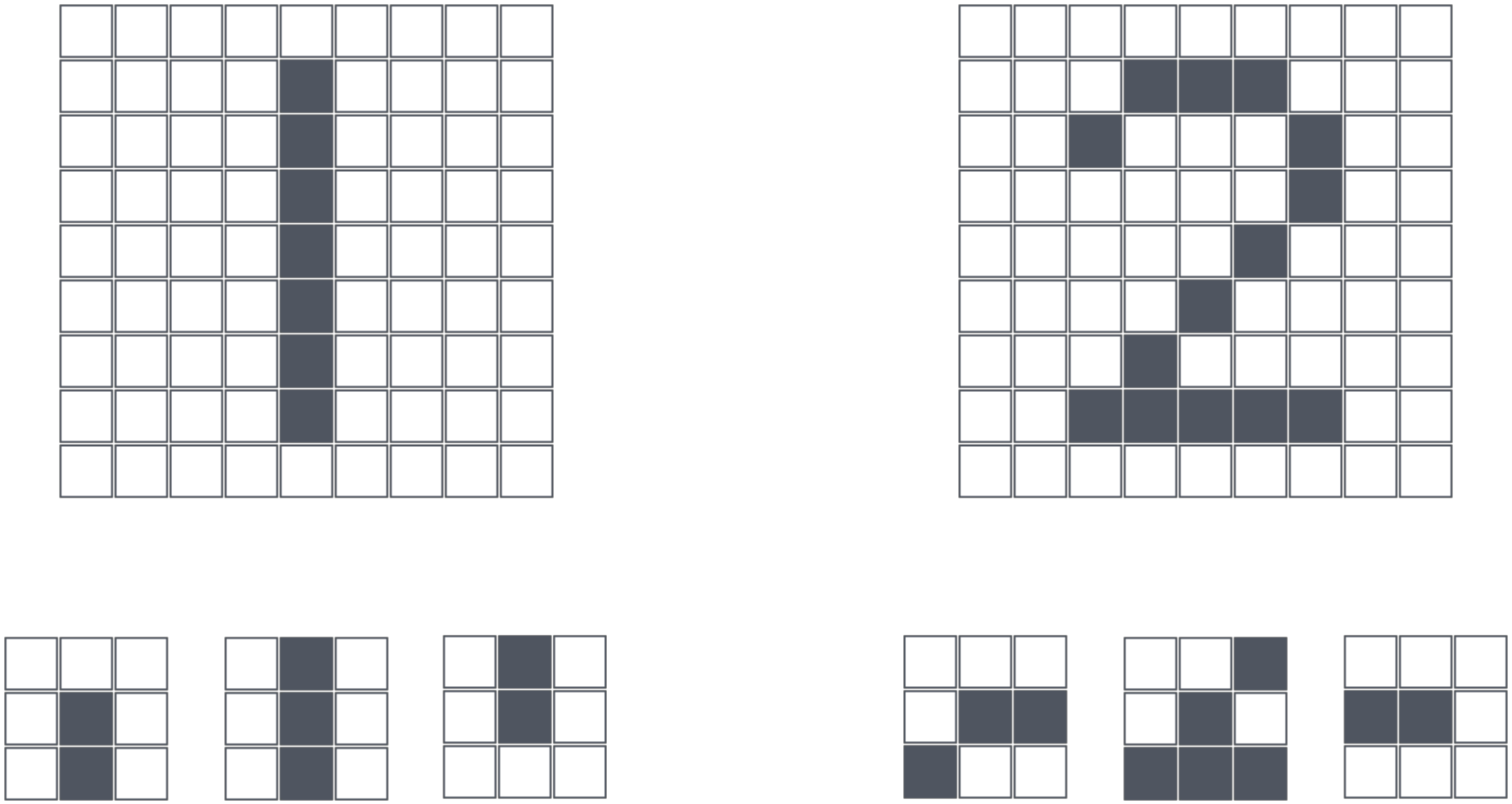
- How can we **identify quantum phases of matter** using ML tools?

- **Convolutional** neural networks



convolutional neural networks

Convolutional neural networks look for **recurring patterns** using small filters.



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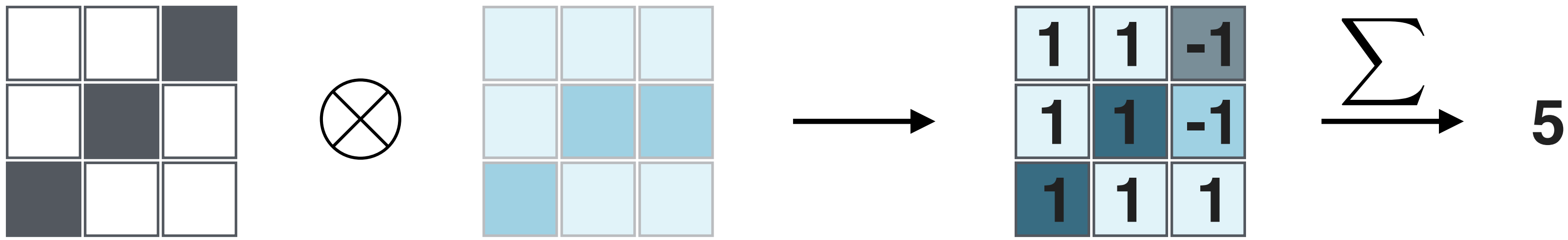

Slide filters across image and create new image based on how well they fit.

convolutional neural networks

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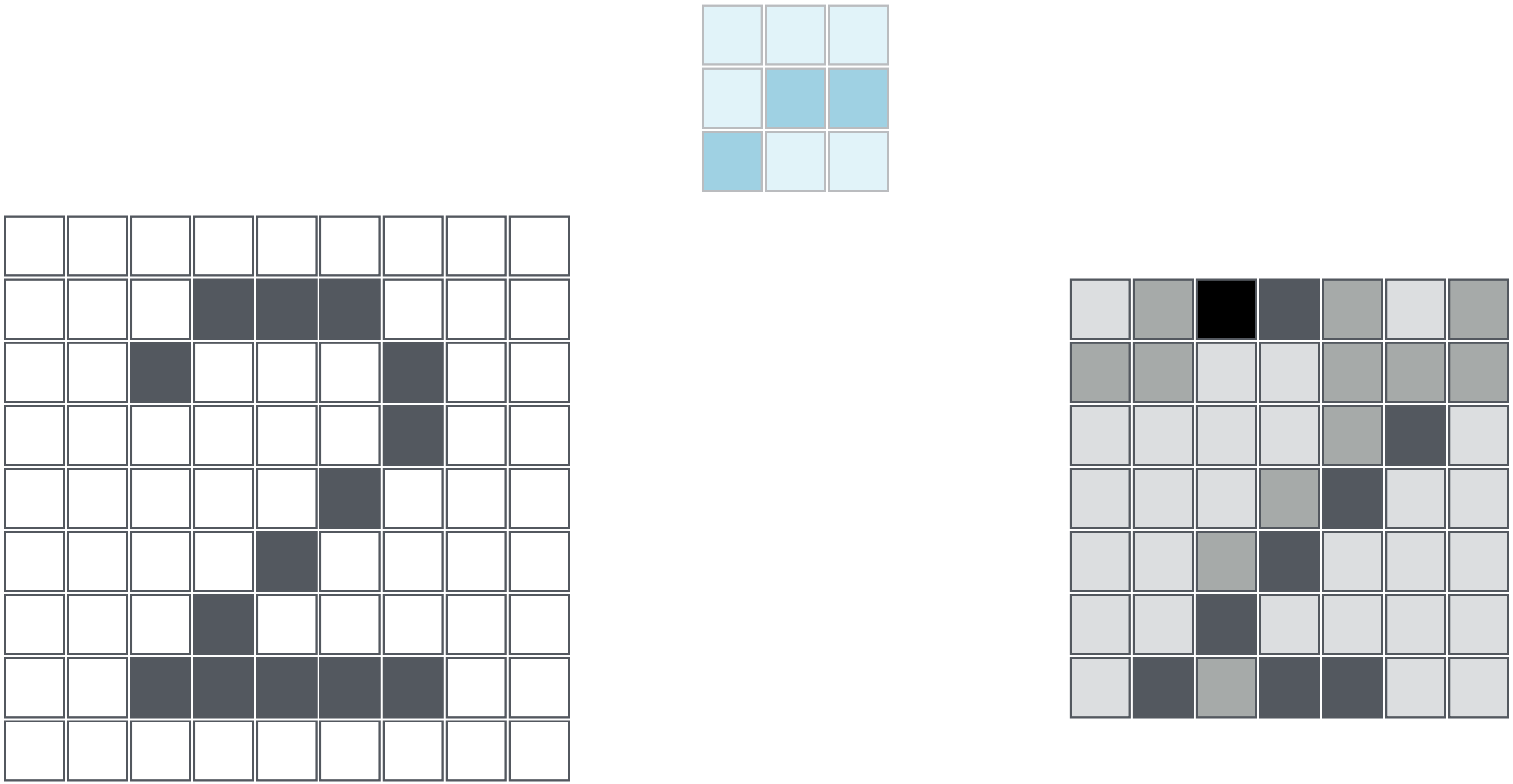


discriminating phases of matter

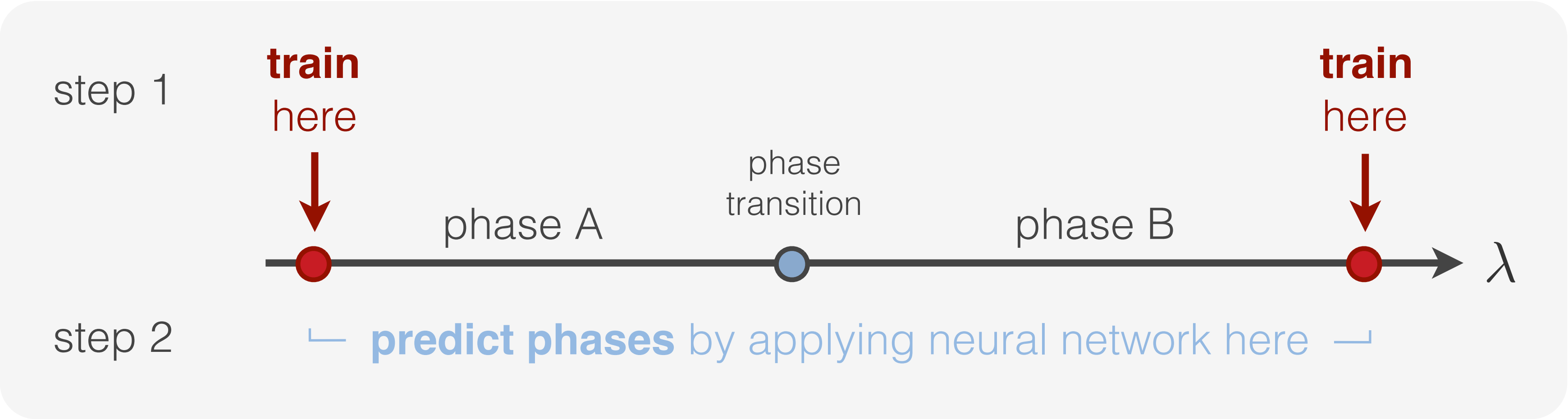
General setup

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

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**

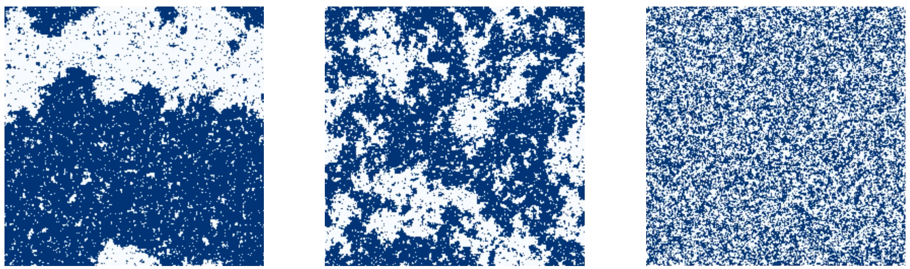


What are the **right images** to feed into the neural network?

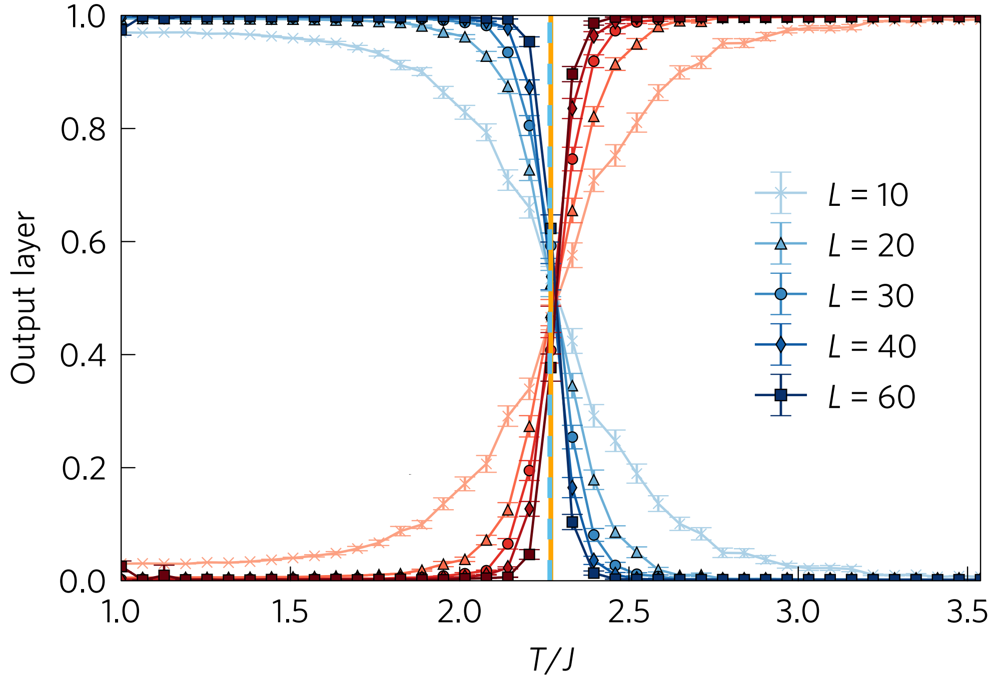
classical phases of matter

Carrasquilla and Melko, Nat. Phys. (2017)

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

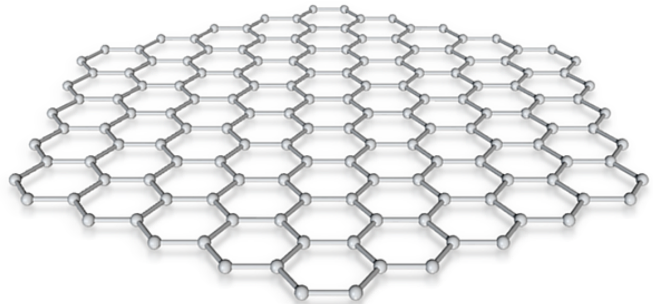


low temperature critical temperature high temperature



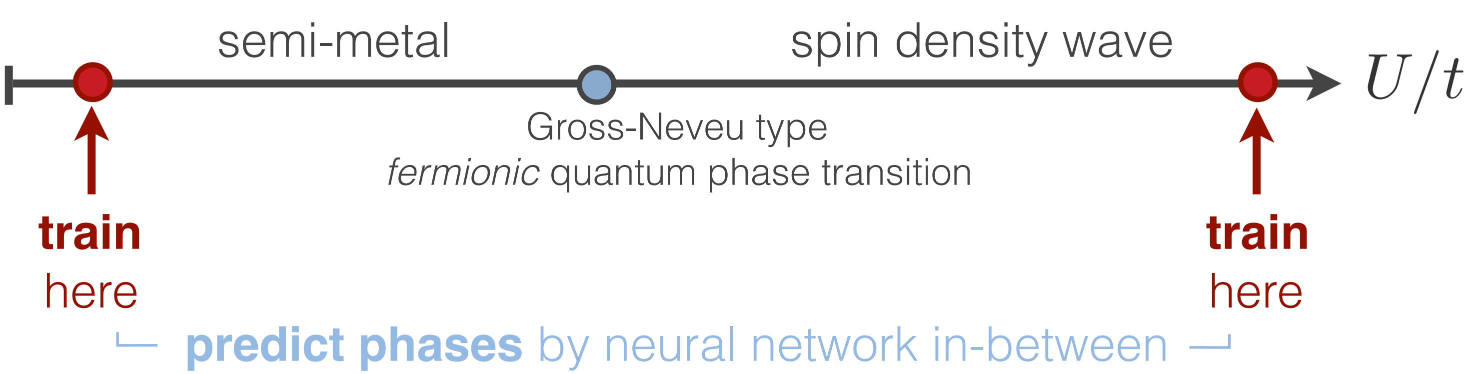
quantum phases of matter

Hubbard models on the honeycomb lattice



Spinful fermions

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



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

quantum phases of matter

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

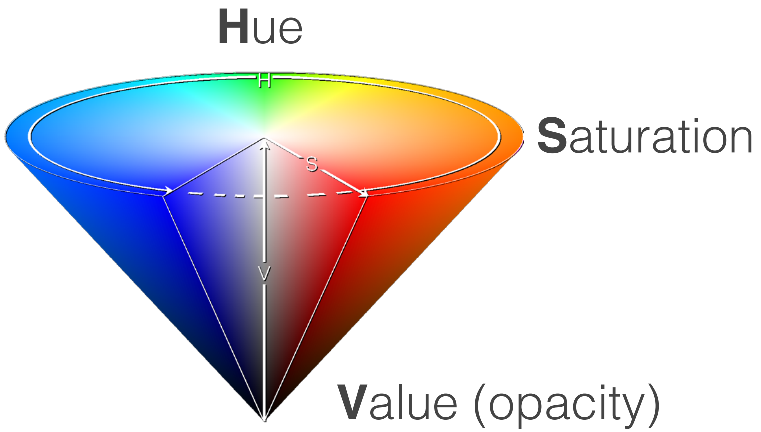
Path integral representation of partition sum

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

Decouple quartic interaction via **Hubbard-Stratonovich** transformation → free fermions in classical background field.

Alternative – **Green's functions**

$$G(i,j) = \langle c_i c_j^\dagger \rangle$$



quantum phases of matter

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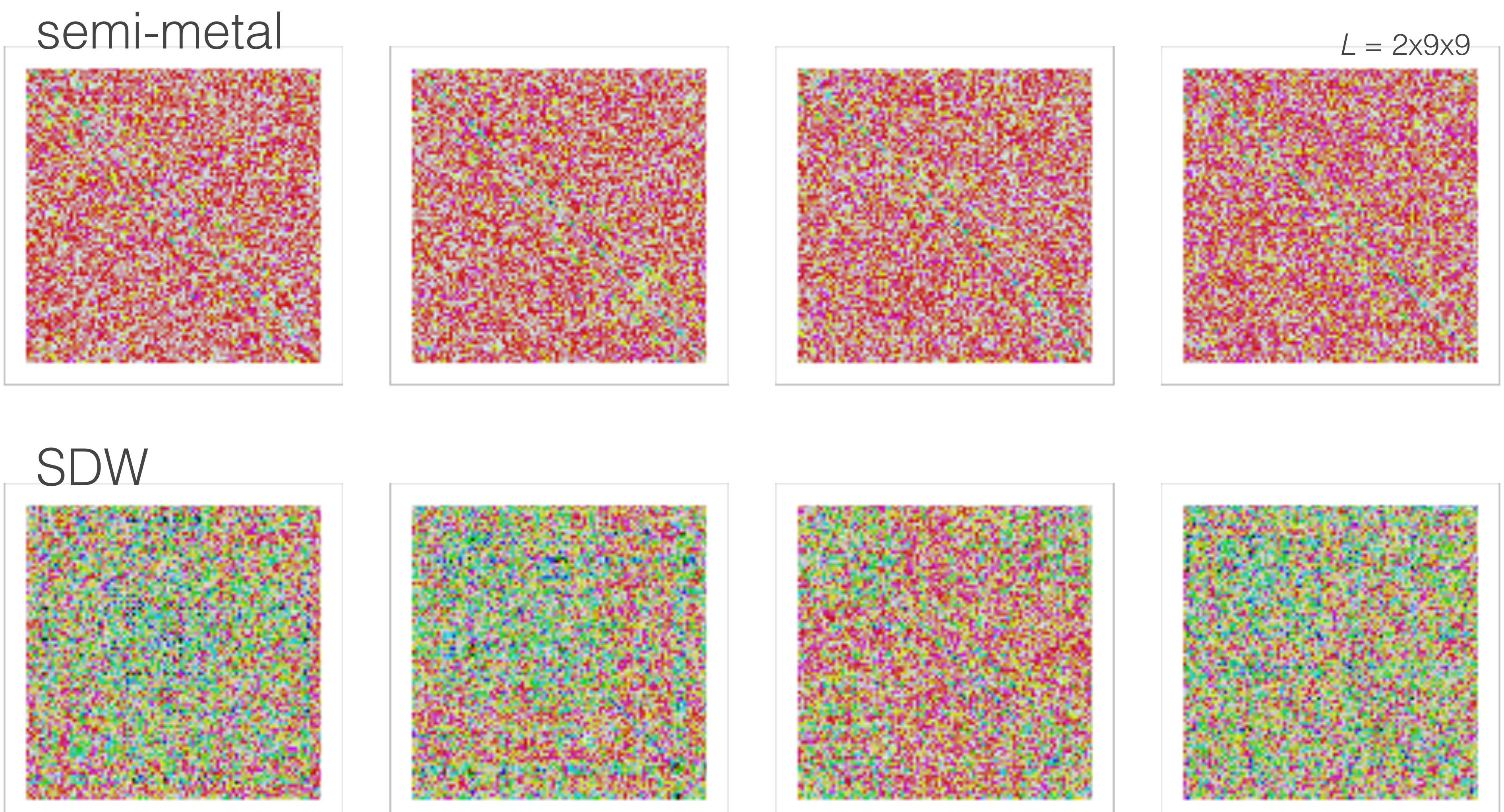
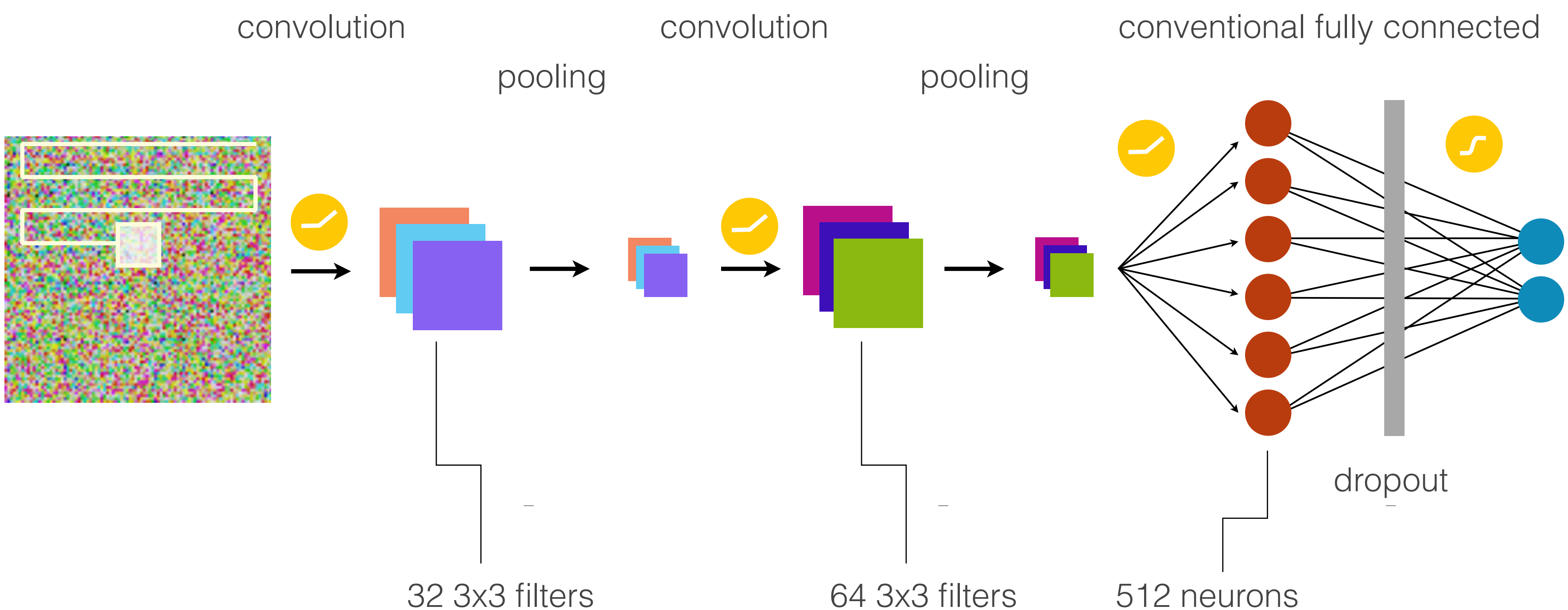
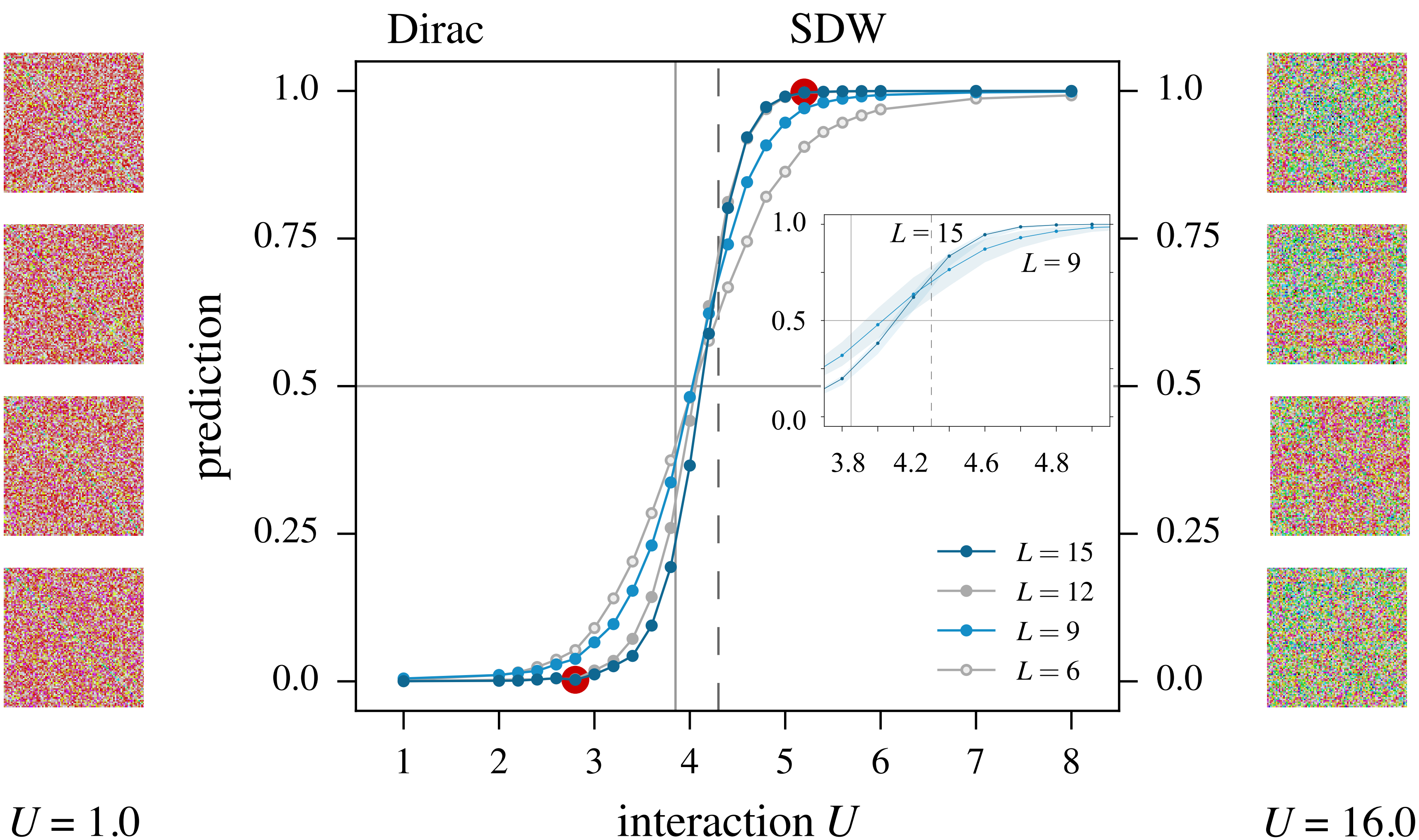


convolutional neural networks



quantum phases of matter

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

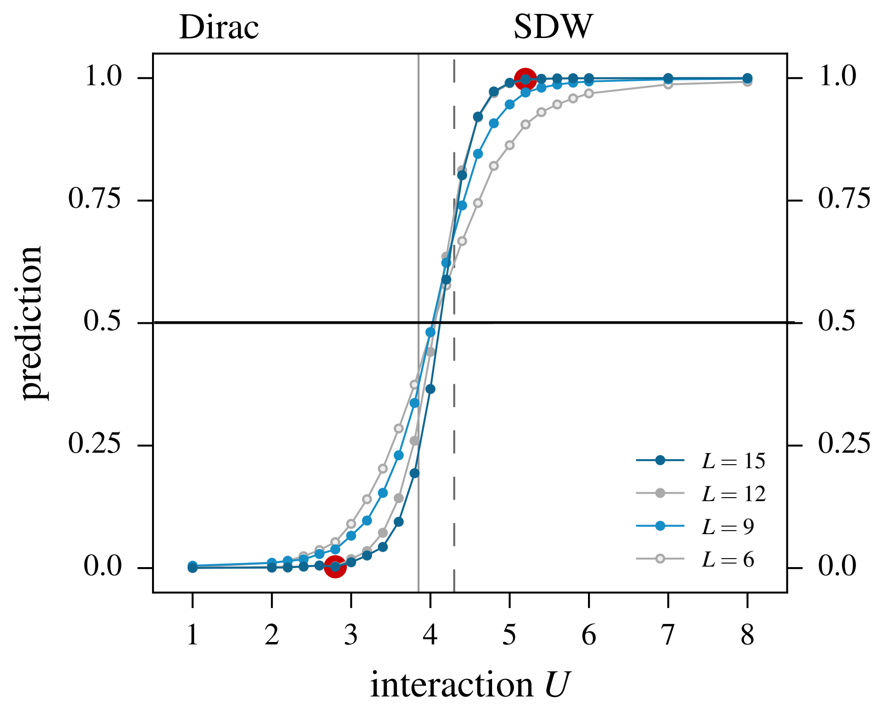


unsupervised approach

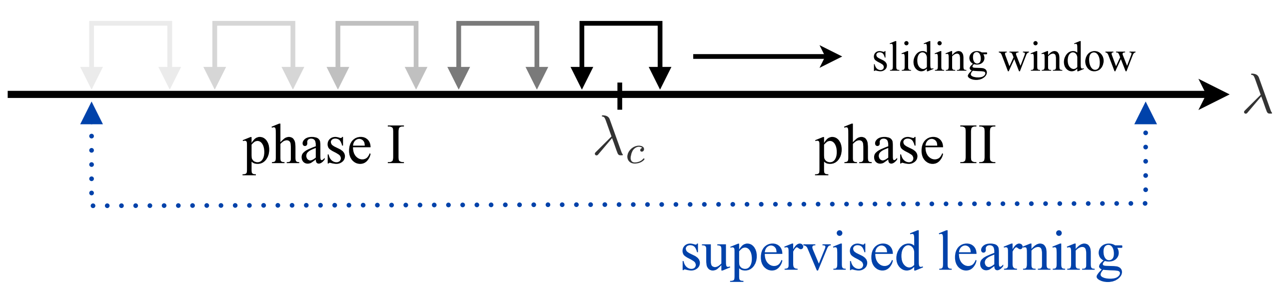
Peter Broecker, Fakher Assaad, ST
arXiv:1707.00663

unsupervised learning

- goal: training with **unlabeled data**
- successful training with **pseudo-labels** itself reveals distinct phases!



- turning supervised learning into unsupervised learning



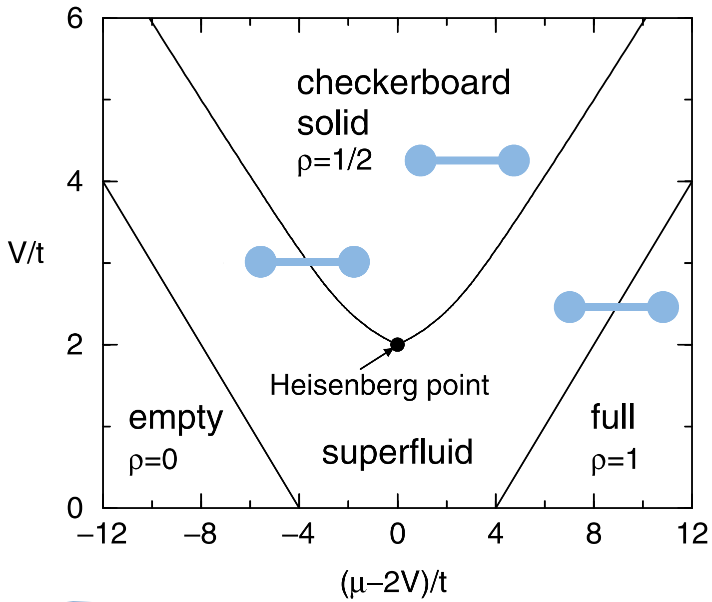
self-learning phase diagrams

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

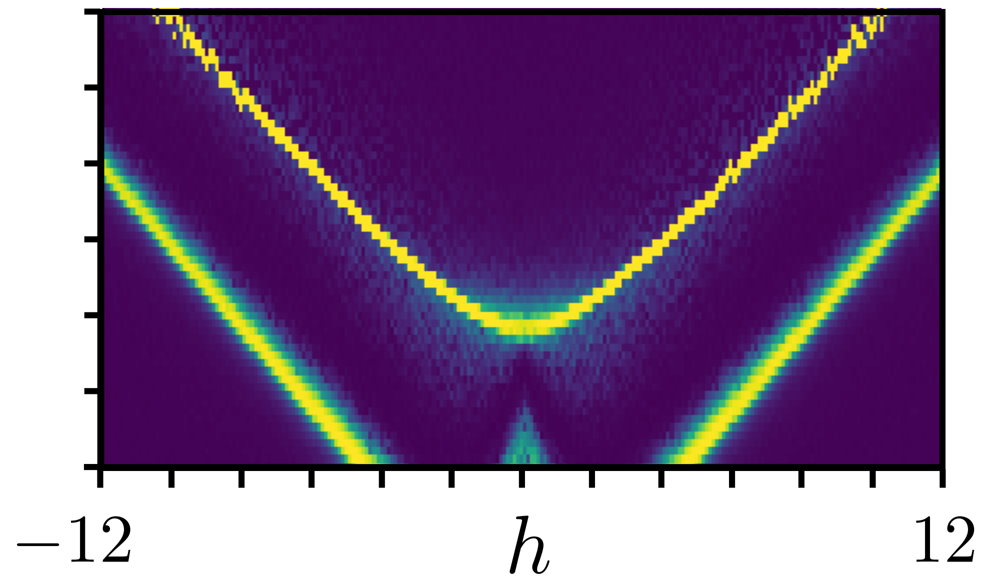
Example: hardcore bosons / XXZ model on a square lattice

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

PRL **88**, 167208 (2002)



$\langle S_i^+ S_j^- \rangle + \langle S_i^- S_j^+ \rangle$ arXiv:1707.00663



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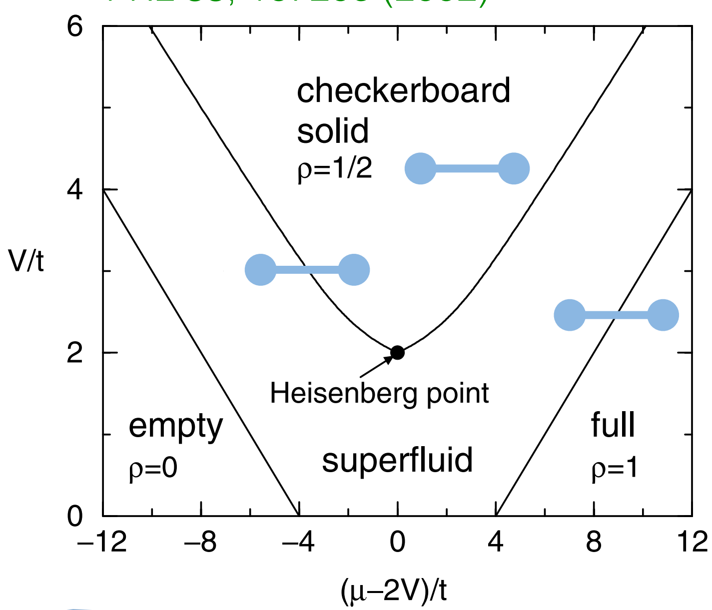

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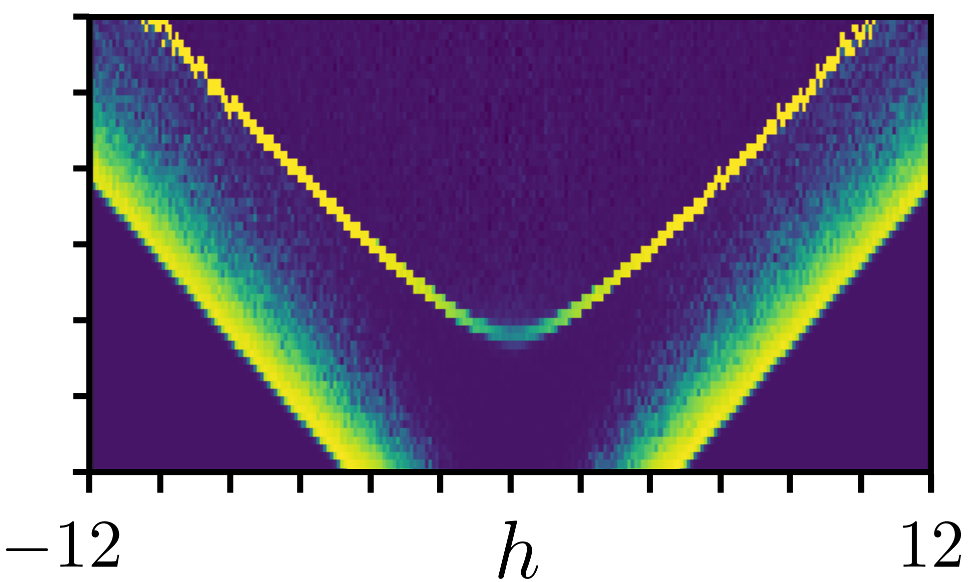

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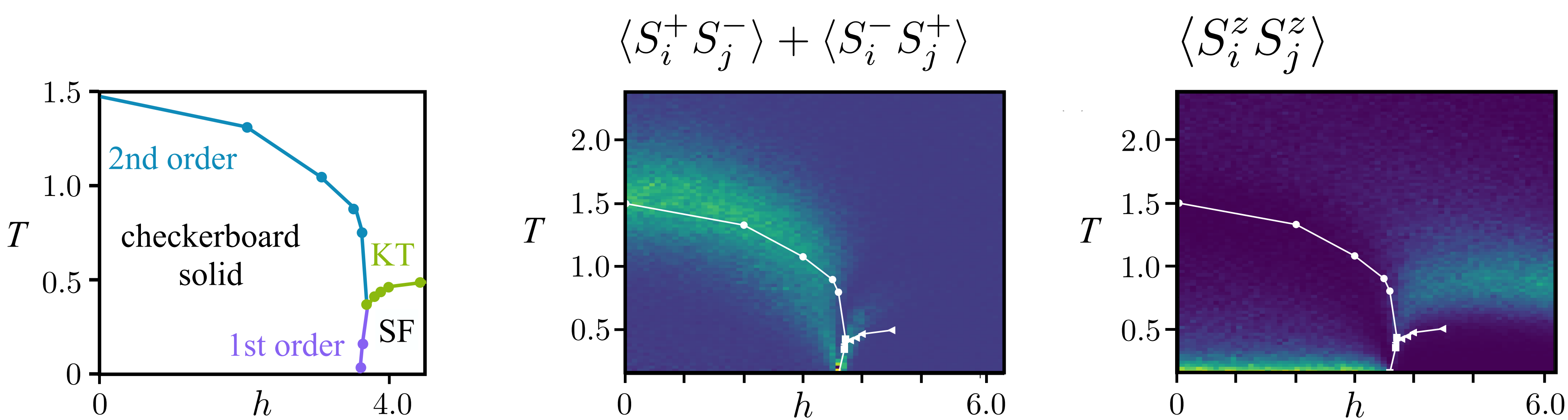


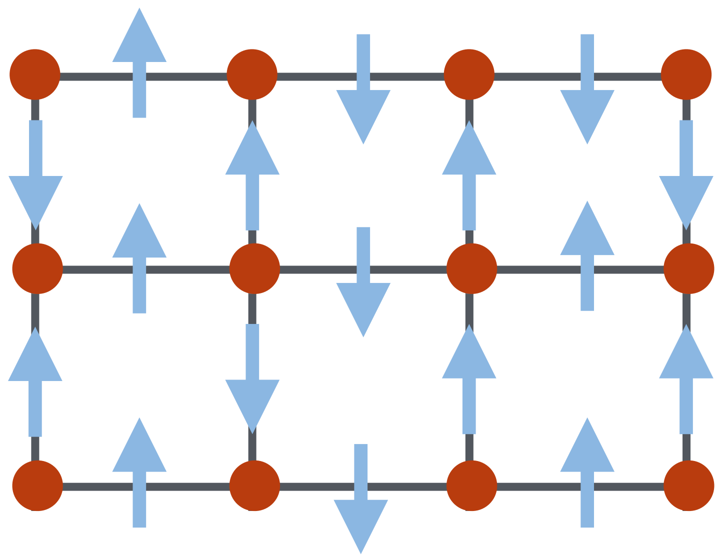
more complex states

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) Z2 (Ising) spins on bonds

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



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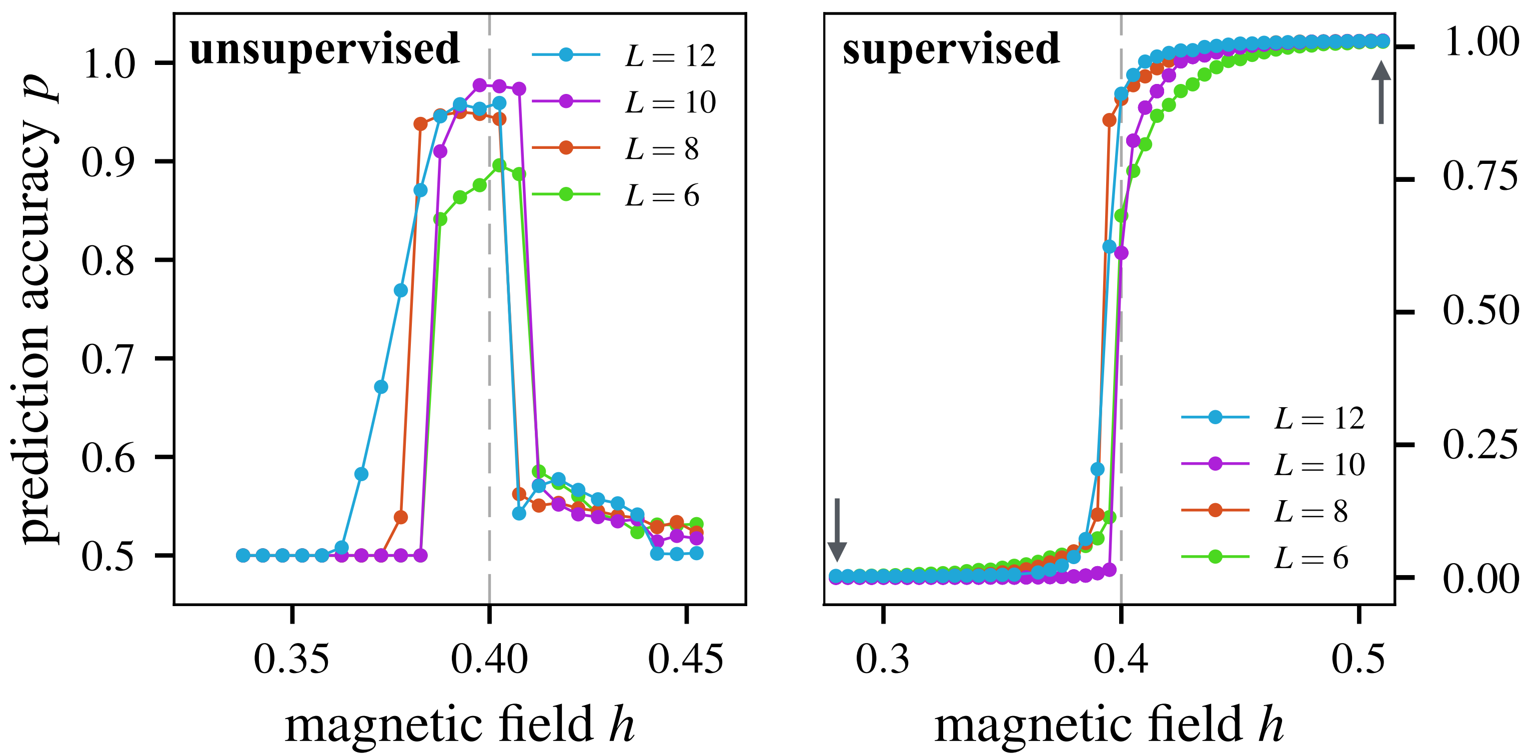


learning transport

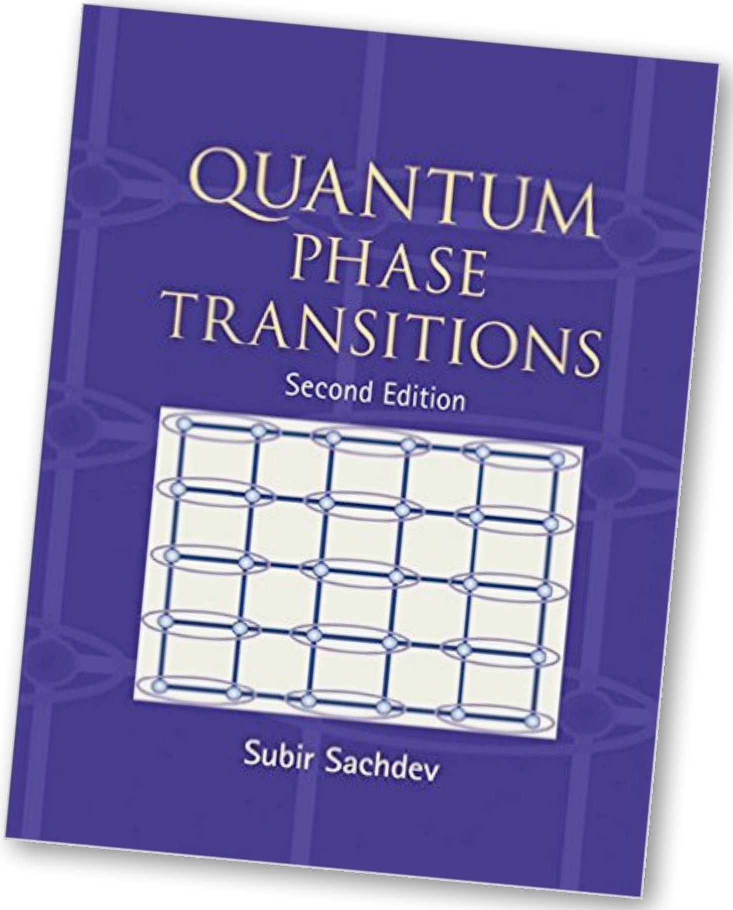
Yi Zhang, C. Bauer, P Broecker, ST, and Eun-Ah Kim
arXiv:1812.05631

Quantum phase transitions

Quantum fluctuations can drive **phase transitions** at zero temperature.

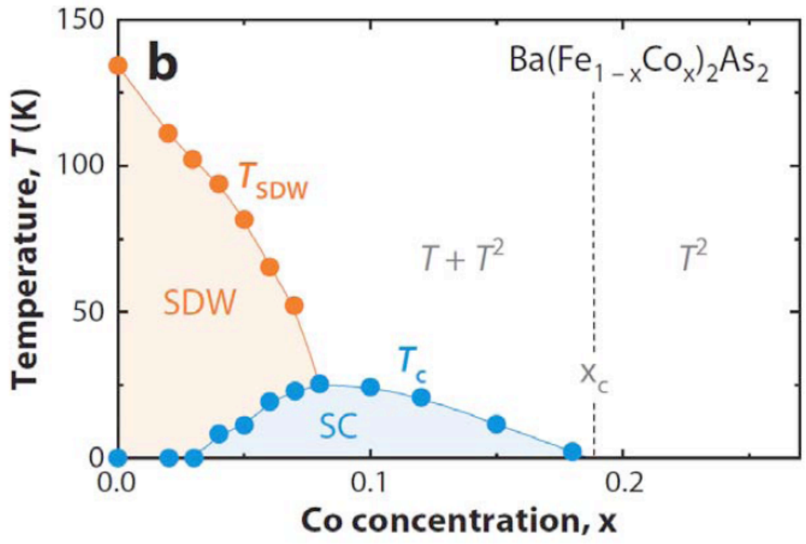
By now such continuous quantum phase transitions are fairly **well understood in insulators**.

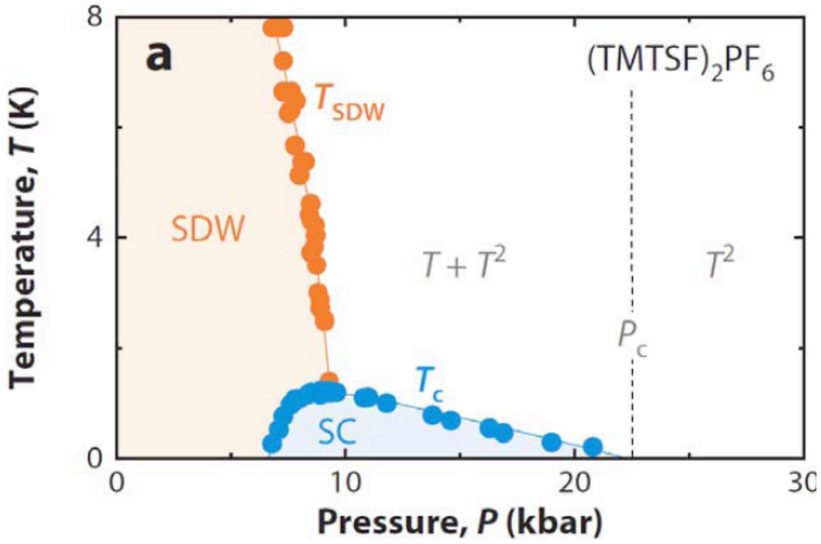
But **what about metals?**
What happens when a system with a Fermi surface goes critical?



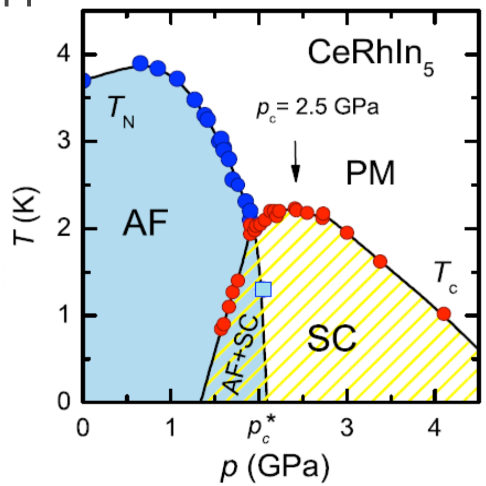
Competing orders in a metal

Fe-based superconductors

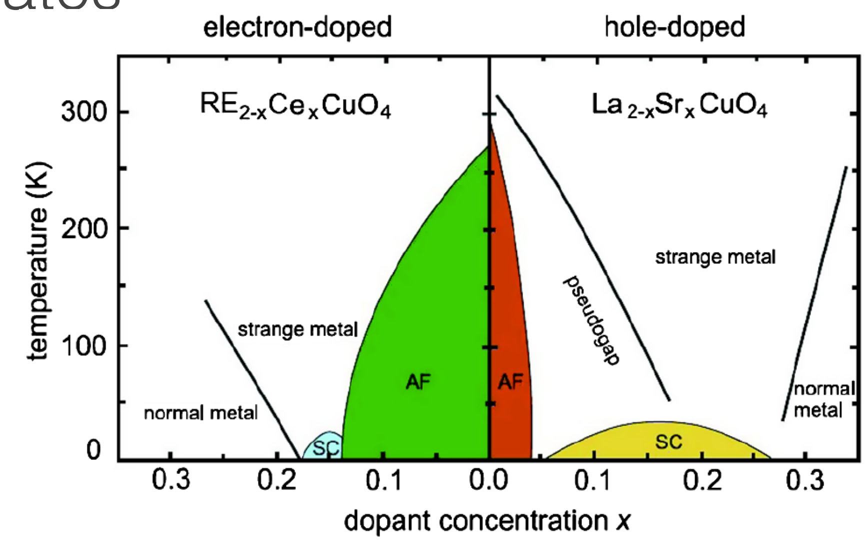




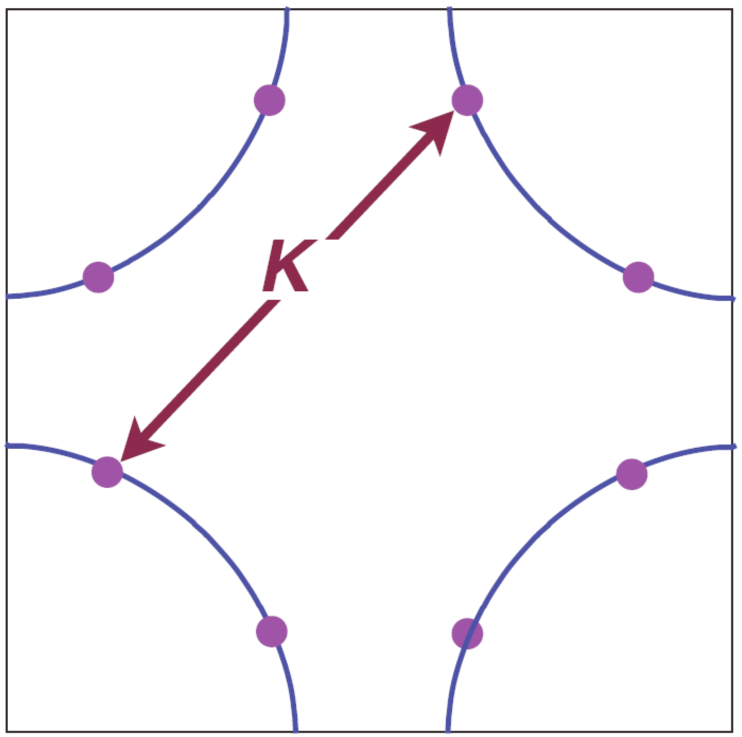
heavy-fermion compounds



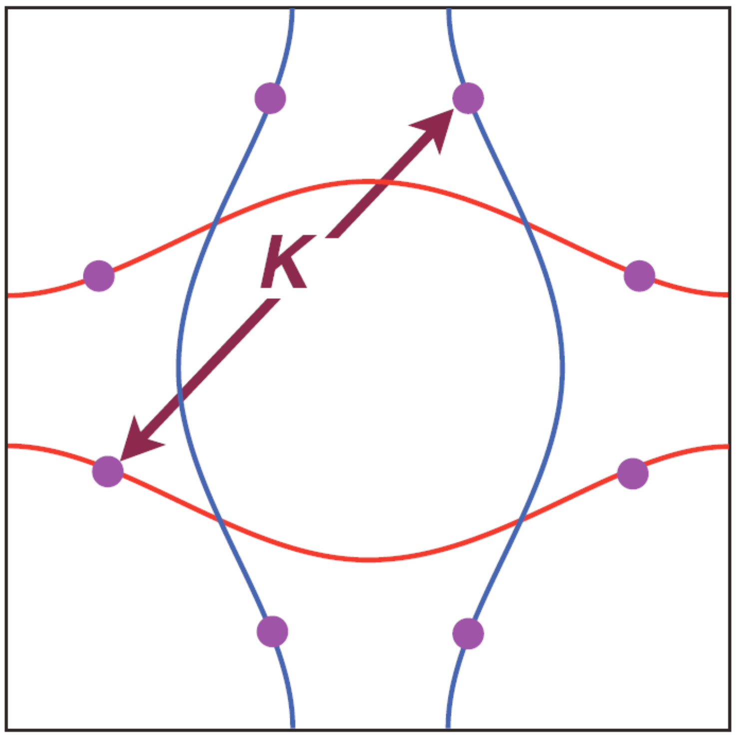
cuprates



Metals 101



Fermi surface with **hot spots**.

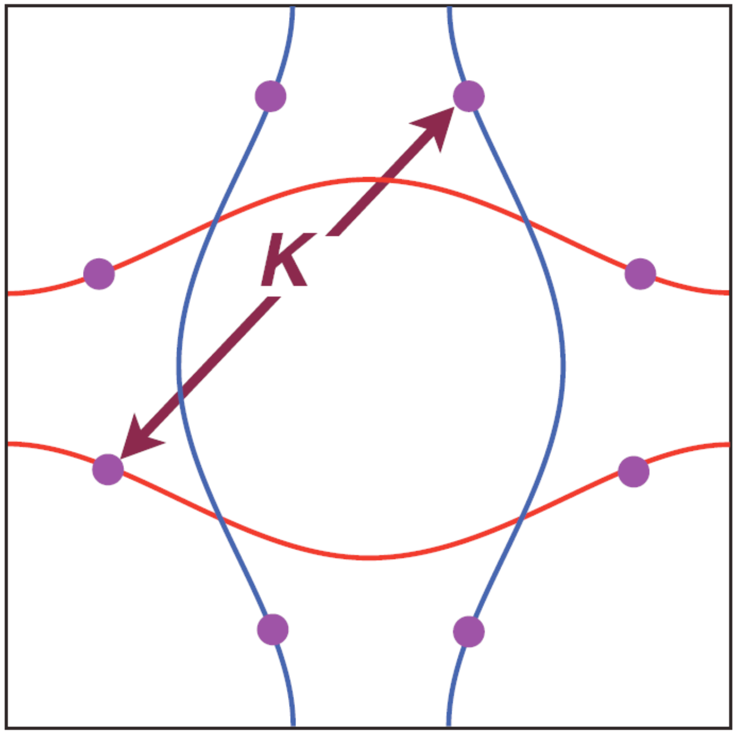


Deformed Fermi surface
away from hot spots.

Faithful representation of low energy theory

Effective “time reversal symmetry”
of the action matrix: **no sign problem**

Competing orders in a metal



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Faithful representation of low energy theory

Effective "time reversal symmetry" of the action matrix: **no sign problem**

Microscopic lattice model

$$S = S_F + S_\varphi = \int_0^\beta \mathrm{d}\tau (L_F + L_\varphi)$$

two fermionic flavors

$$L_F = \sum_{\substack{i,j,s\\ \alpha=x,y}} \psi^\dagger_{\alpha i s} \left[(\partial_\tau - \mu)\delta_{ij} - t_{\alpha ij}\right] \psi_{\alpha j s}$$

$$+ \lambda \sum_{i,s,s'} e^{i\mathbf{Q}\cdot\mathbf{r}_i} [\vec{s}\cdot\vec{\varphi}_i]_{ss'} \psi^\dagger_{xis}\psi_{yis'} + \text{h.c.}$$

SDW coupling

bosonic O(2) order parameter

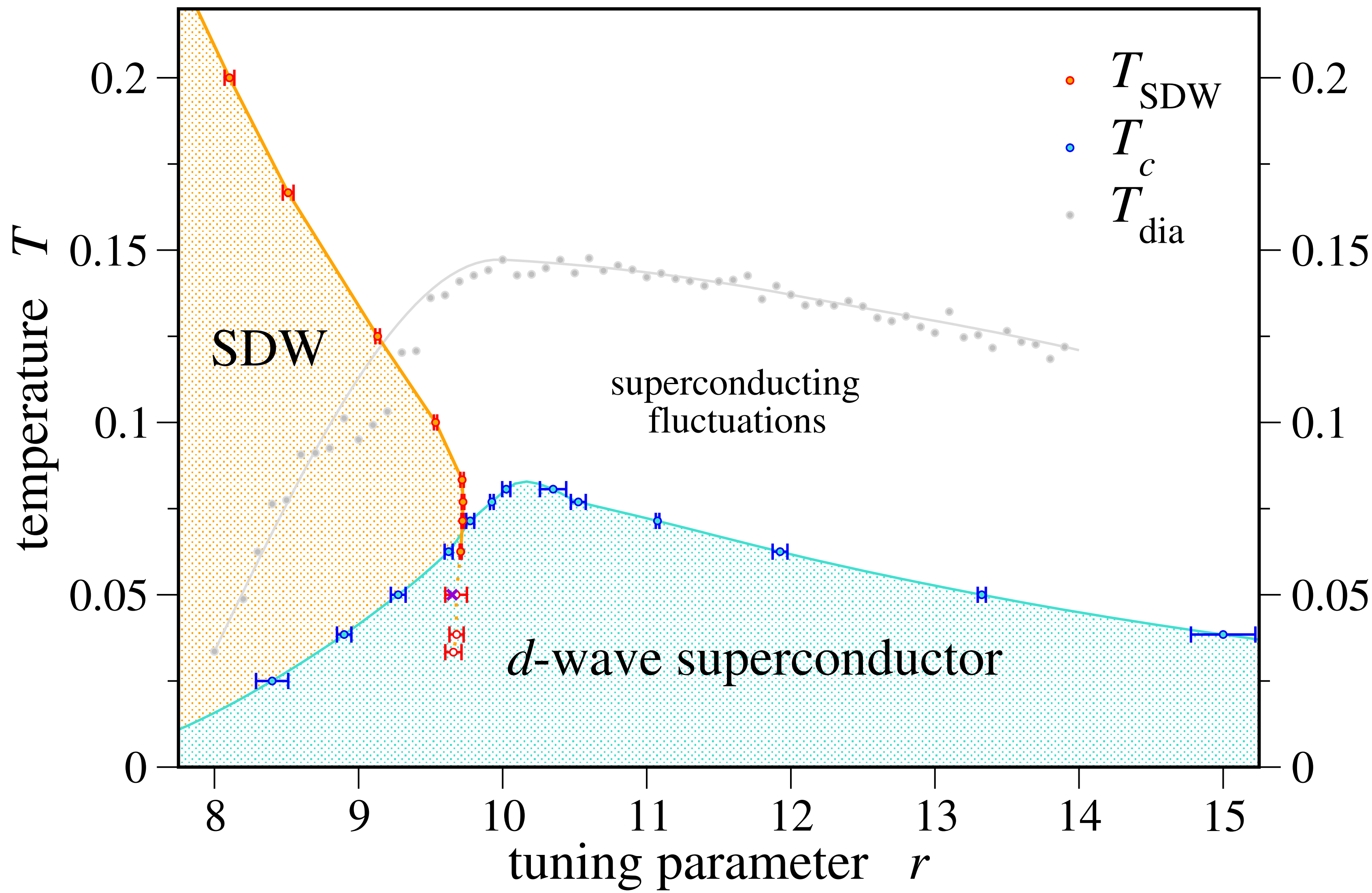
$$L_\varphi = \frac{1}{2}\sum_i \frac{1}{c^2}\left(\frac{\mathrm{d}\vec{\varphi}_i}{\mathrm{d}\tau}\right)^2 + \frac{1}{2}\sum_{\langle i,j\rangle}(\vec{\varphi}_i - \vec{\varphi}_j)^2$$

$$+ \sum_i \left[\frac{r}{2}\vec{\varphi}_i^2 + \frac{u}{4}(\vec{\varphi}_i^2)^2\right].$$

tuning parameter

Competing orders in a metal

Y Schattner, M. Gerlach, ST, E. Berg, PRL (2016)
Ann. Rev. Cond. Matt. Physics (2019)



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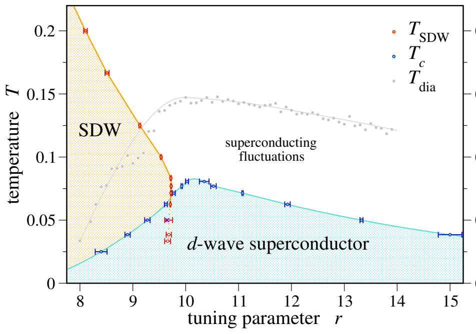
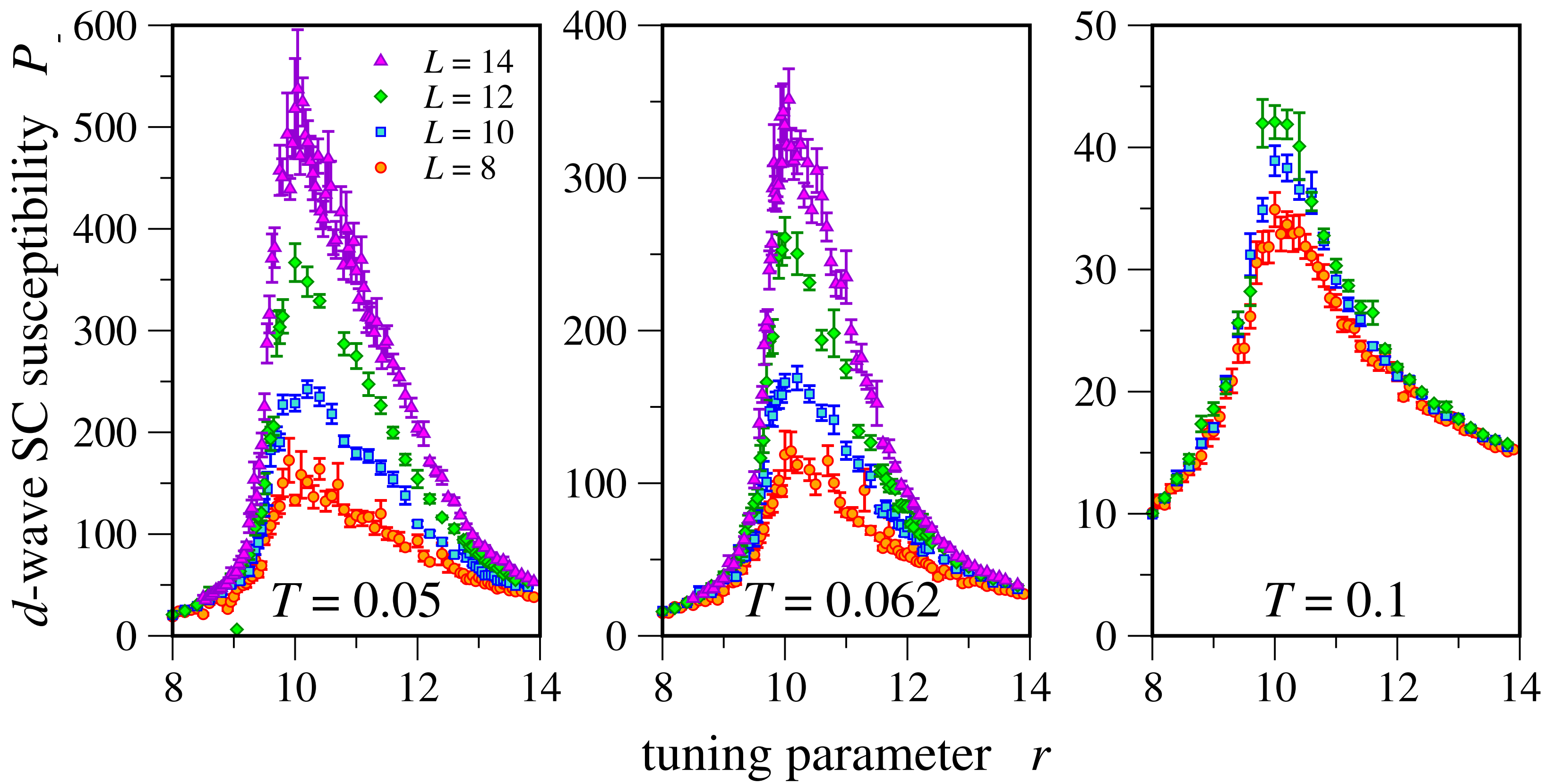


The superconducting phase exhibits **d-wave pairing**, signaled by a *diverging* d-wave pairing susceptibility.

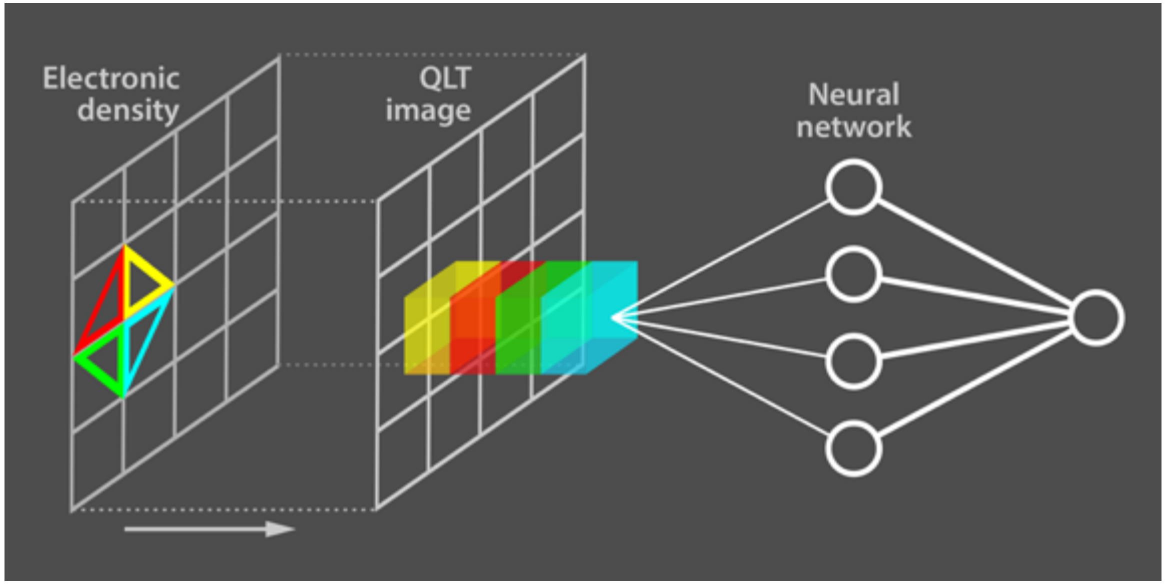
$$P_- = \int d\tau \sum_i \langle \Delta_-^\dagger(\mathbf{r}_i, \tau) \Delta_-(\mathbf{0}, 0) \rangle \qquad \Delta_-(\mathbf{r}_i) = \psi_{xi\uparrow}^\dagger \psi_{xi\downarrow}^\dagger - \psi_{yi\uparrow}^\dagger \psi_{yi\downarrow}^\dagger$$



machine learning superconductivity

Yi (Frank) Zhang and Eun-Ah Kim, PRL (2017)

Quantum loop topography is a physics preprocessor allowing to identify features associated with topological order in quantum many-body systems.



$$\tilde{P}_{jk}\tilde{P}_{kl}\tilde{P}_{lj}$$

$$\tilde{P}_{jk} \equiv \left\langle c_j^\dagger c_k \right\rangle_\alpha$$

↓

$$\int d\tau \left\langle \hat{j}_x(\mathbf{r}_1,\tau)\,\hat{j}_x(\mathbf{r}_2,0)\right\rangle$$

↓

proxy for longitudinal transport

Quantum loop = sample of two-point operators that form loops.

superconductivity

Yi Zhang, C. Bauer, P. Broecker, ST & Eun-Ah Kim, arXiv:1812.05631

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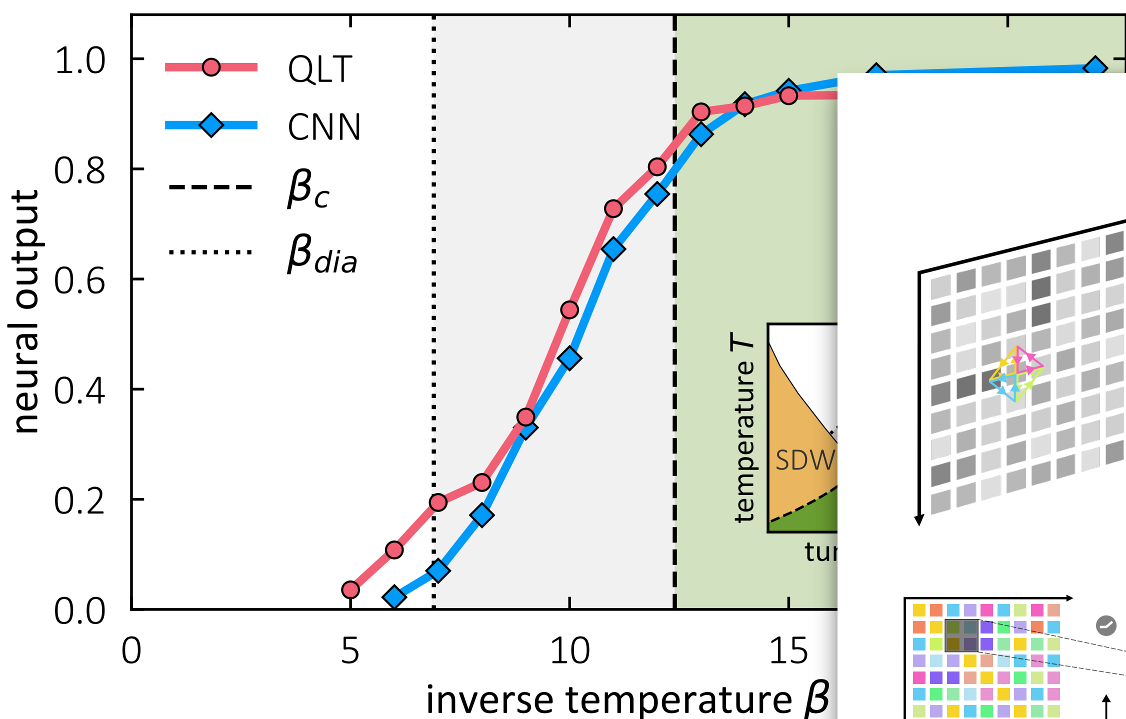

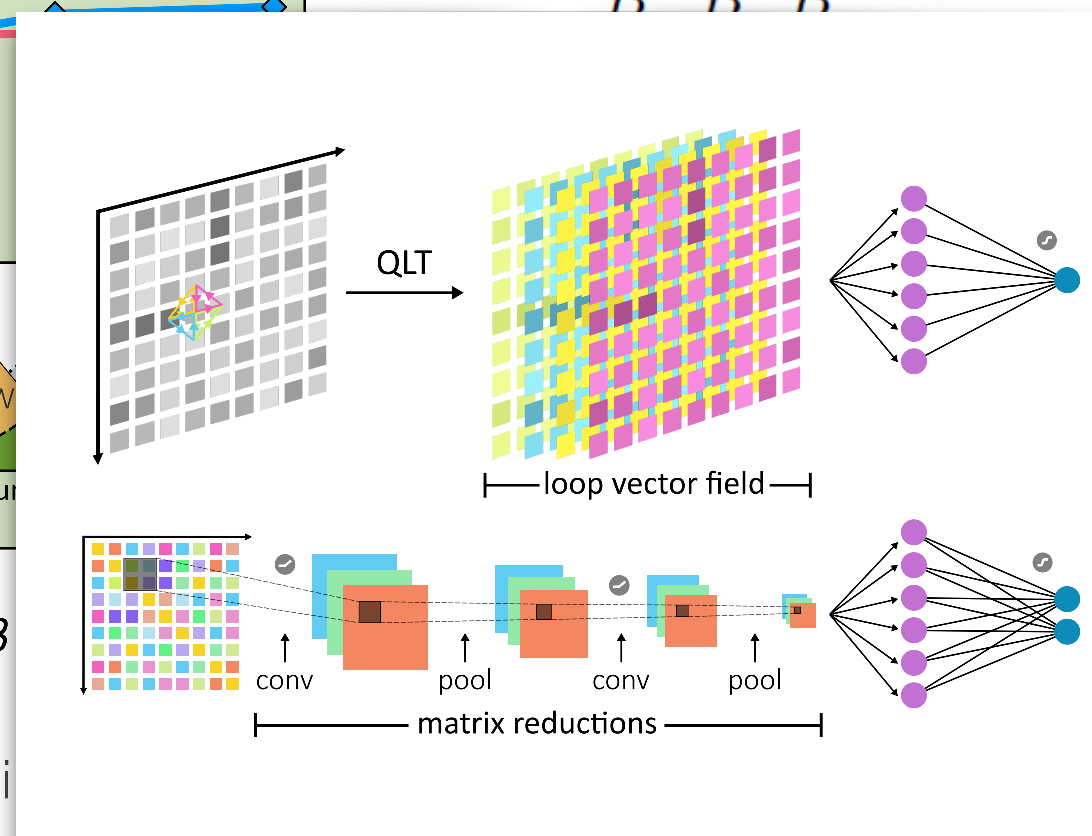

Quantum loop = sample of two-poi

superconductivity

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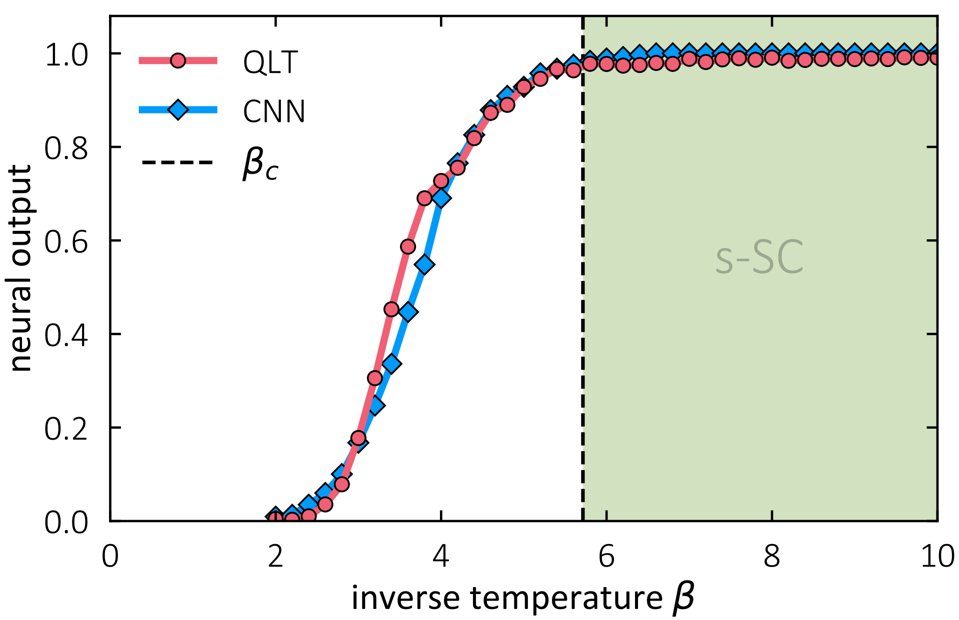
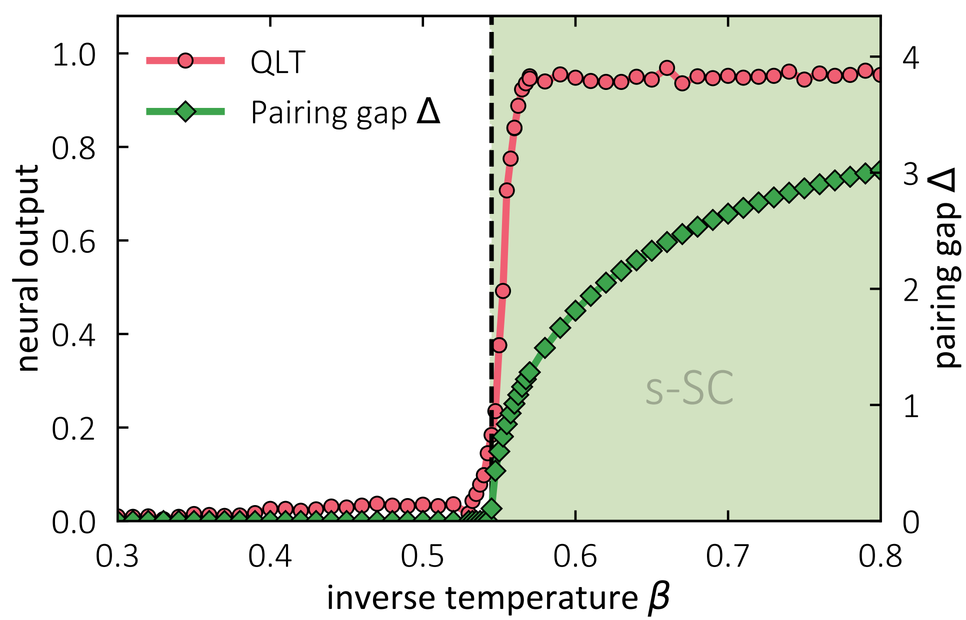


negative-U Hubbard model



mean-field transition

spin-fermion model

Y Schattner, M. Gerlach, ST, E. Berg, PRL (2016)
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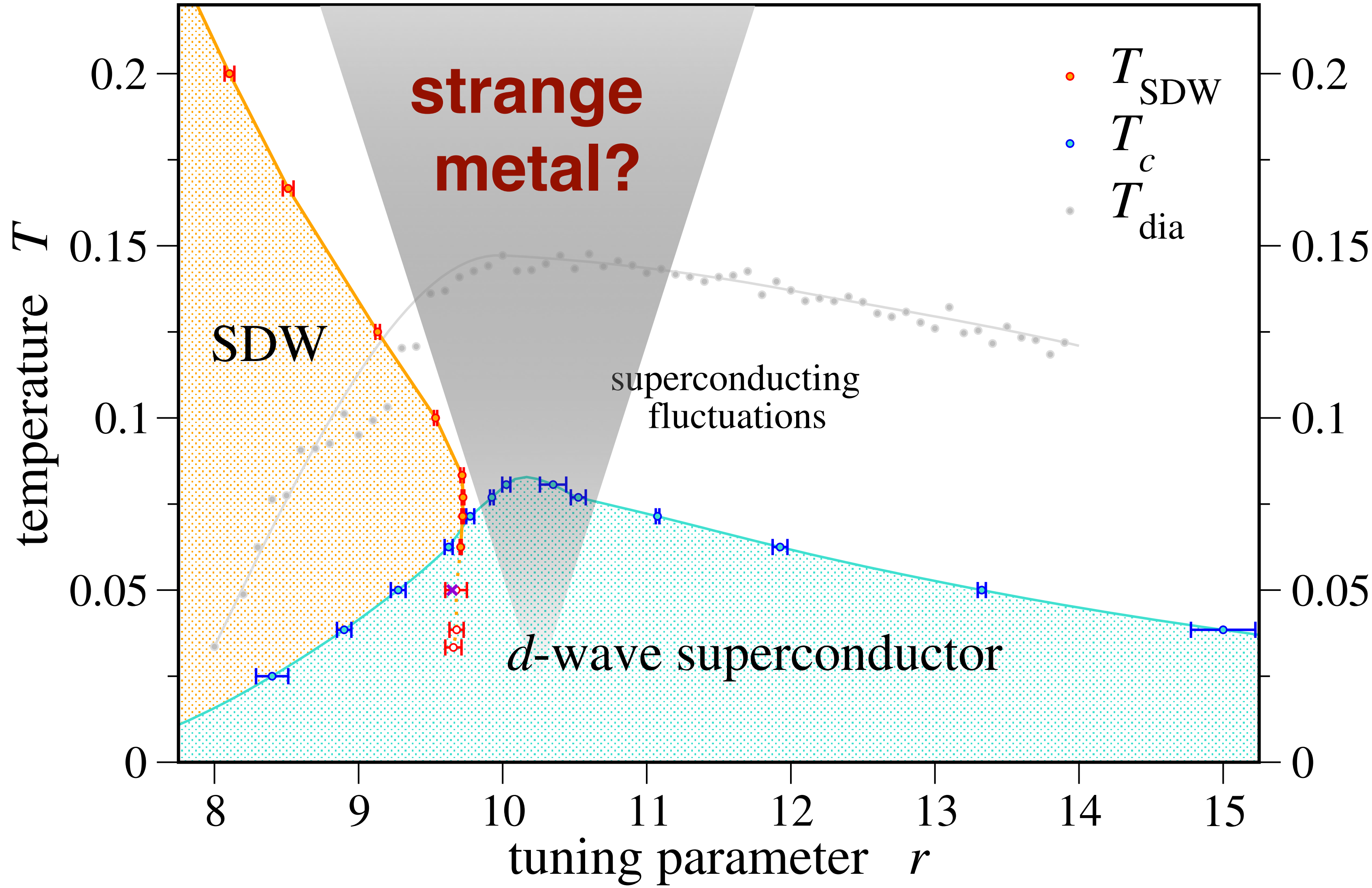
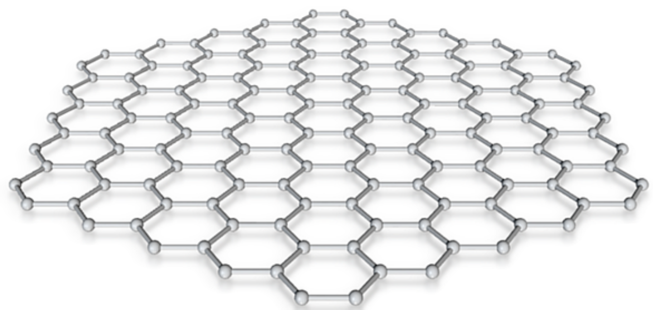


sign problem
+ machine learning

Peter Broecker, Juan Carrasquilla, Roger G. Melko, ST
Scientific Reports (2017)

spinless Dirac matter

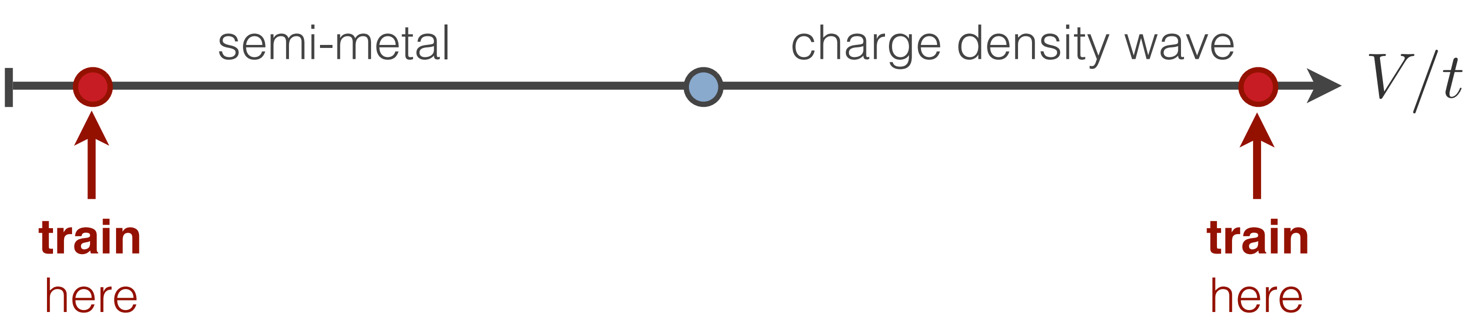
Hubbard models on the honeycomb lattice



Spinless fermions

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

severe sign problem



└ **predict phases** by neural network in-between ┘

One way out — basis transformation to **Majorana fermions**.
But let's go the hard way …

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**

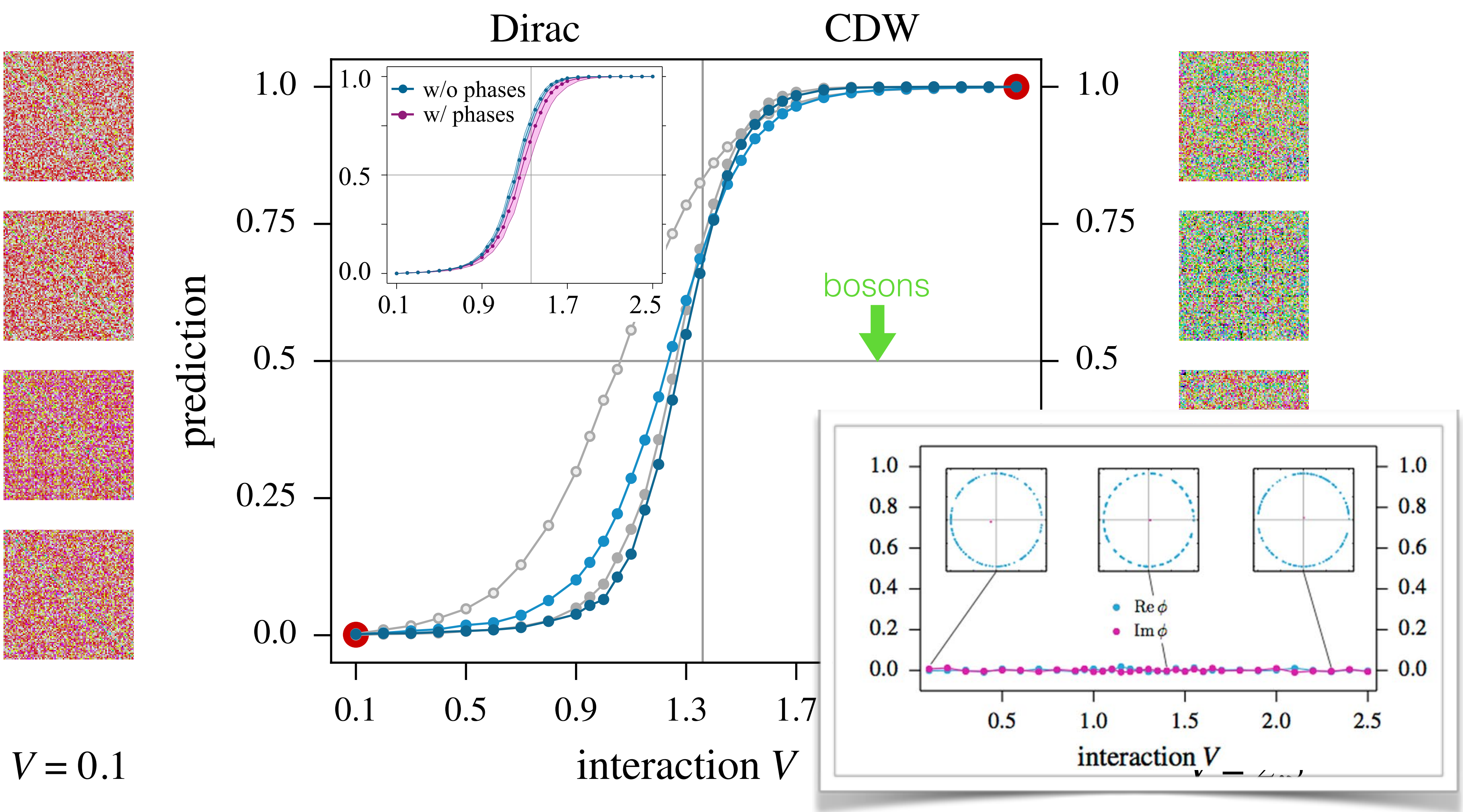
Assume there exists a "state function"

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

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**.



summary

Summary

QMC + machine learning approach can be used to distinguish phases of interacting classical and quantum many-body systems.

- unsupervised learning of phase diagrams
- new opportunities to circumvent the fermion sign problem.
- improve data handling with new physics filters

arXiv:1812.05631
arXiv:1707.00663
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