

Title: Machine learning quantum phases of matter beyond the fermion sign problem

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Abstract:

Machine Learning of Quantum Phases of Matter Beyond the Fermion Sign Problem

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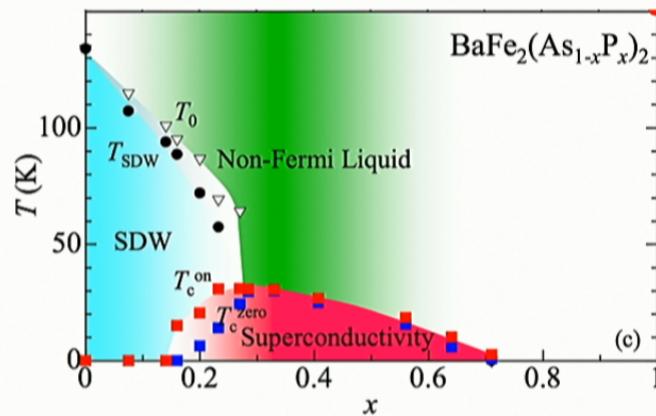
Simon Trebst

Cologne



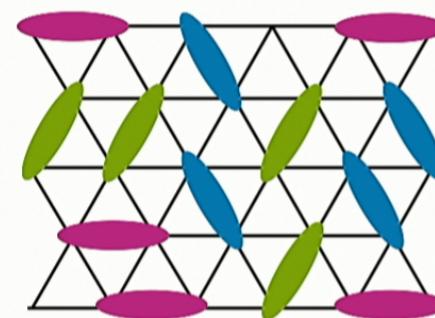
Quantum phases of matter

Correlated many fermion systems exhibit some of the most intriguing phases of quantum matter



many-electron systems
superconductivity

[image from Sachdev and Keimer, Physics Today, 2011]



frustrated magnets
quantum spin liquids

Numerical simulations of quantum matter

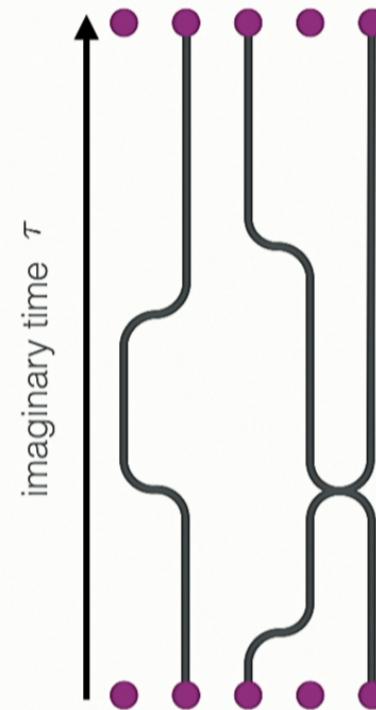
Quantum Monte Carlo simulations
mapping a **quantum** to a **classical** problem

Sample the quantum **partition function**

$$\mathcal{Z} = \text{Tr } e^{-\beta \mathcal{H}}$$

via **world-line** configurations
to calculate expectation values

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



The sign problem

There can be negative weights ...

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positive definite weight
fluctuating observable

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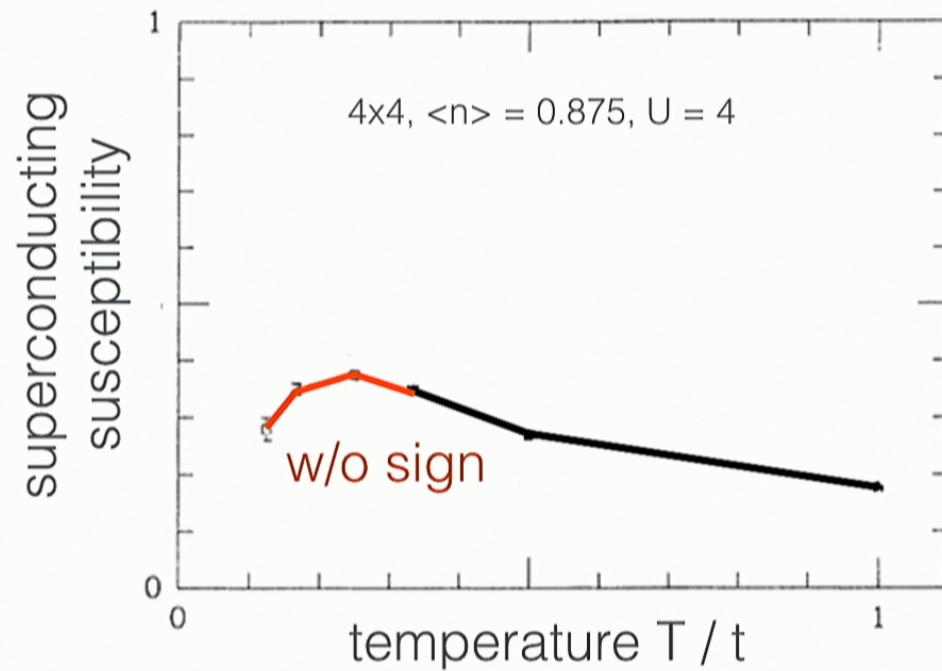
... but the average sign decreases exponentially

$$\langle \sigma \rangle = \frac{\sum |\sigma(\mathcal{C})| |p(\mathcal{C})|}{\sum |p(\mathcal{C})|} = \frac{Z}{Z_{|p|}} = e^{-\beta N \Delta f}$$

Is the sign really important?

classic example: superconductivity in doped Hubbard model

[Loh, Gubernatis, Scalettar, White, Scalapino and Sugar, PRB 1990]



correlation functions come out wrong!

Circumventing the sign problem

Sign problem is **basis dependent**

energy eigenbasis \longleftrightarrow simulation basis
also **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 - the sign problem is NP hard

[Troyer and Wiese, PRL 2005]

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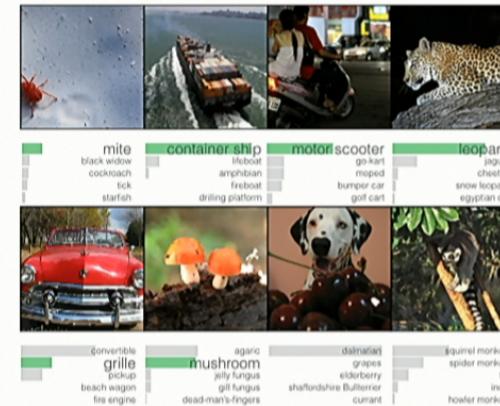
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Machine learning perspective

Convolutional neural networks have proved to be extremely powerful ingredients to pattern recognition/machine learning.



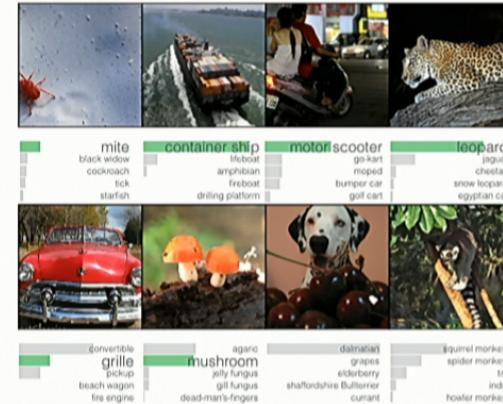
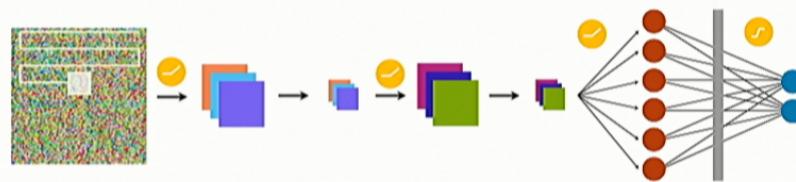
adapted from [AlexNet 2012]

Can we adapt machine learning approaches to circumvent the sign problem in quantum Monte Carlo simulations?

Which physical quantity contains sufficient information to serve as input for pattern recognition approaches?

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Quantum Monte Carlo for fermions

[Blankenbecler, Scalapino, Sugar, PRD 1981]

Determinantal QMC is the workhorse for **unbiased** studies of strongly interacting fermion systems.

Access to ground state wave function by projection

$$|\psi\rangle = \lim_{\theta \rightarrow \infty} e^{-\theta\mathcal{H}} |\psi_T\rangle \quad \mathcal{H} = \mathcal{K} + \mathcal{V}$$

$$e^{-\theta\mathcal{H}} |\psi_T\rangle = \prod_{n=1}^{N_\tau} e^{-\Delta\tau\mathcal{K}} e^{-\Delta\tau\mathcal{V}} |\psi_T\rangle$$

Decouple quartic interaction using **Hubbard-Stratonovich** transformation introducing **auxiliary fields**.

Note: There are many different choices here (decoupling channels, symmetries) which result in different types of **real or complex valued auxiliary fields**.

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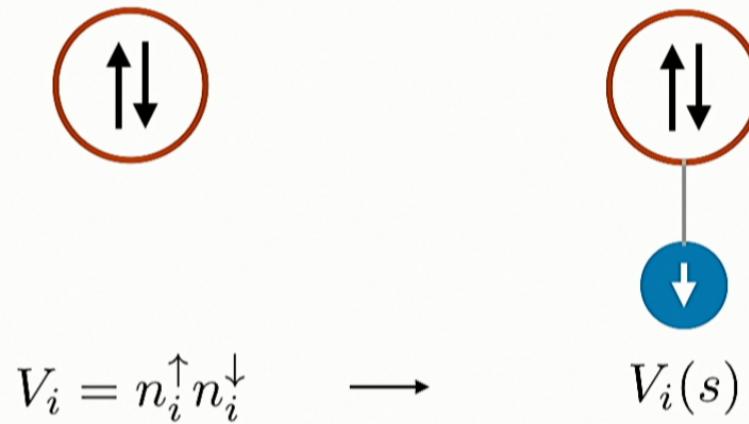
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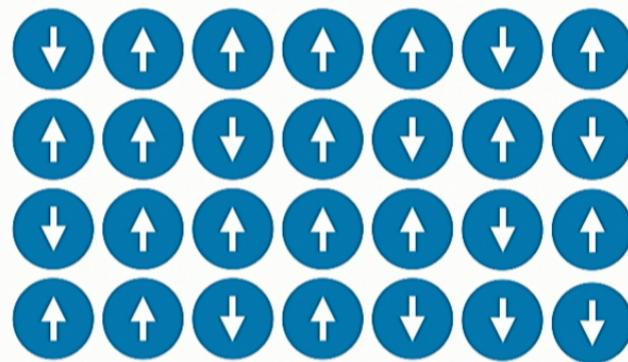
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Decoupling per site



Quantum Monte Carlo for fermions

Hubbard Stratonovich field can be interpreted as image

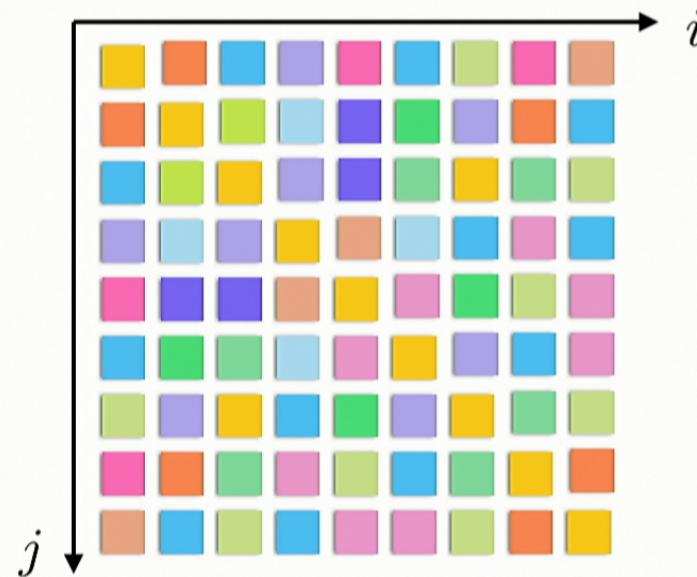


Green's functions

The Green's function $G(i, j) = \langle c_i c_j^\dagger \rangle$ is a fundamental object in quantum statistical mechanics, e.g. allowing for the calculation of equal-time correlation functions.

It is also integral part of the DQMC approach.

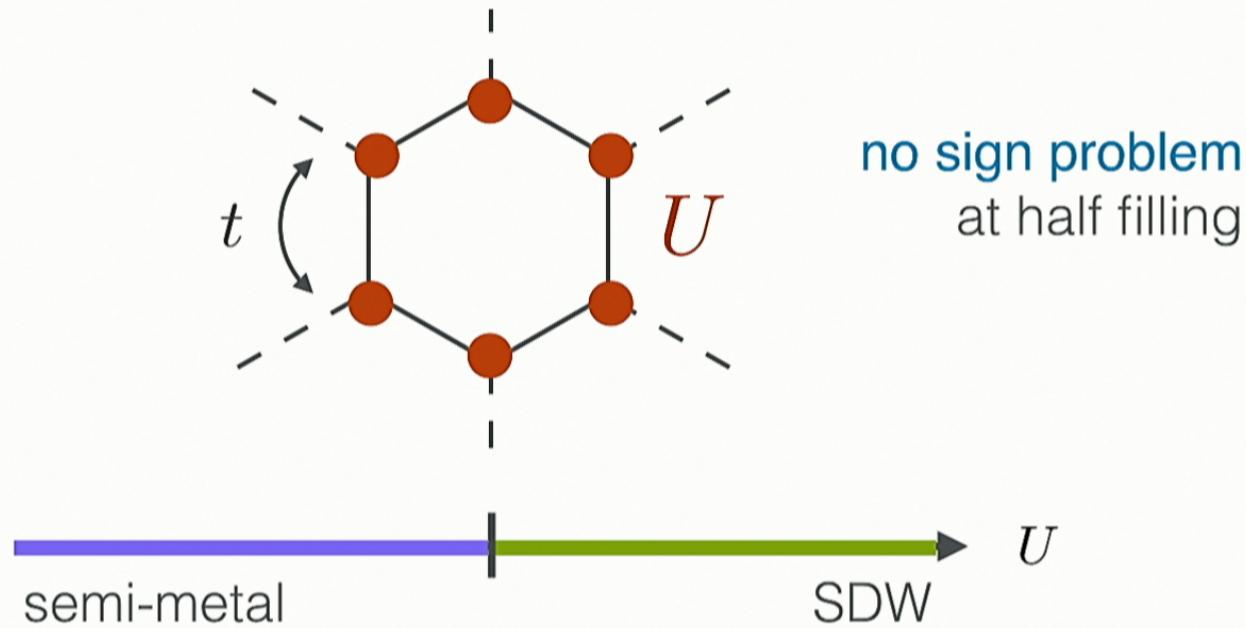
$G(i, j)$ has natural image interpretation



Competing phases for spinful fermions

Interacting spinful fermions on the honeycomb lattice

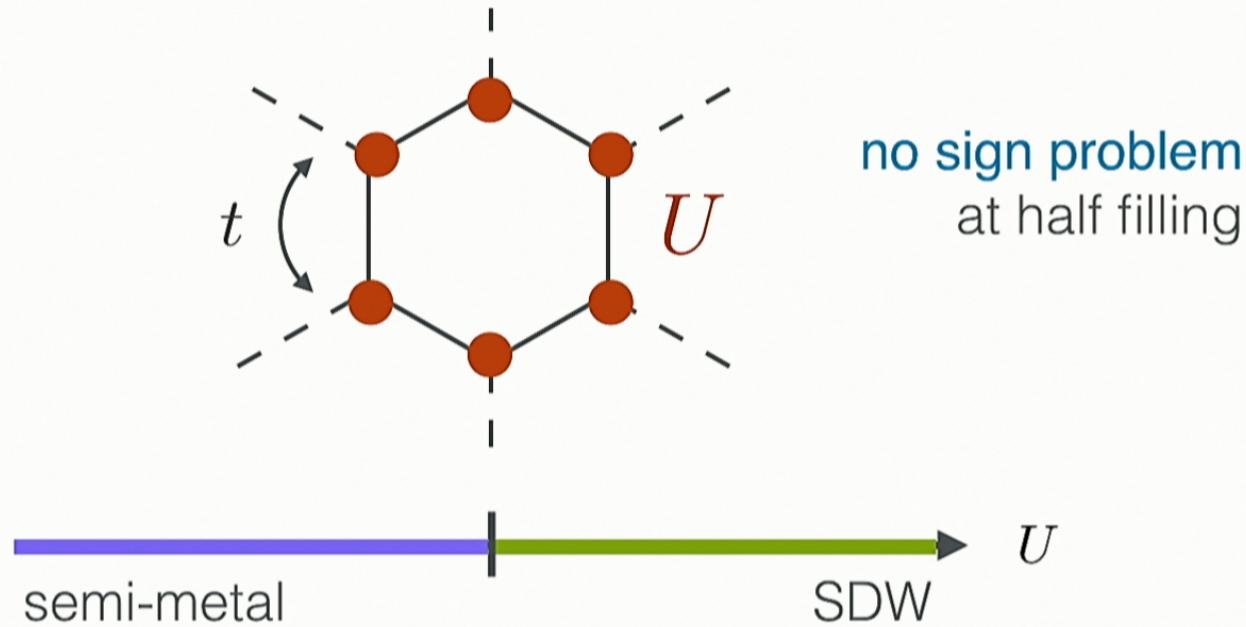
$$H = - \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



Competing phases for spinful fermions

Interacting spinful fermions on the honeycomb lattice

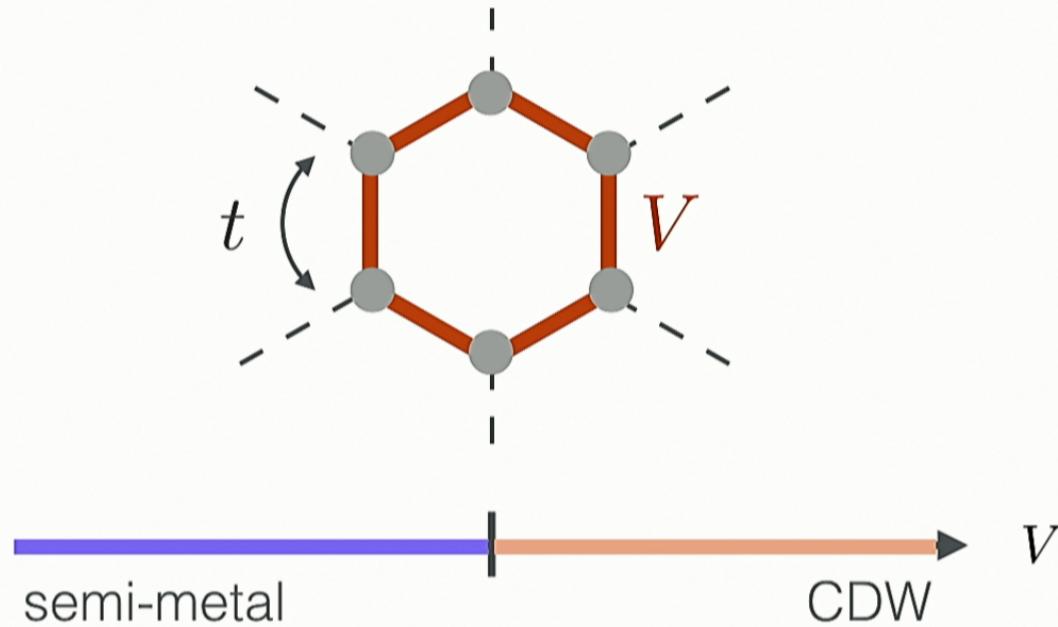
$$H = - \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



Competing phases for spineless fermions

consider interacting fermions on the honeycomb lattice

spinless $H = \sum_{\langle i,j \rangle} -t c_i^\dagger c_j + V n_i n_j$ **severe sign problem**



Supervised learning / auxiliary fields

Case 1: Spinful Fermions

choice of Hubbard Stratonovich transformation influences
image

coupling to ...

magnetization
breaks SU(2)



SM



SDW

charge
preserves SU(2)



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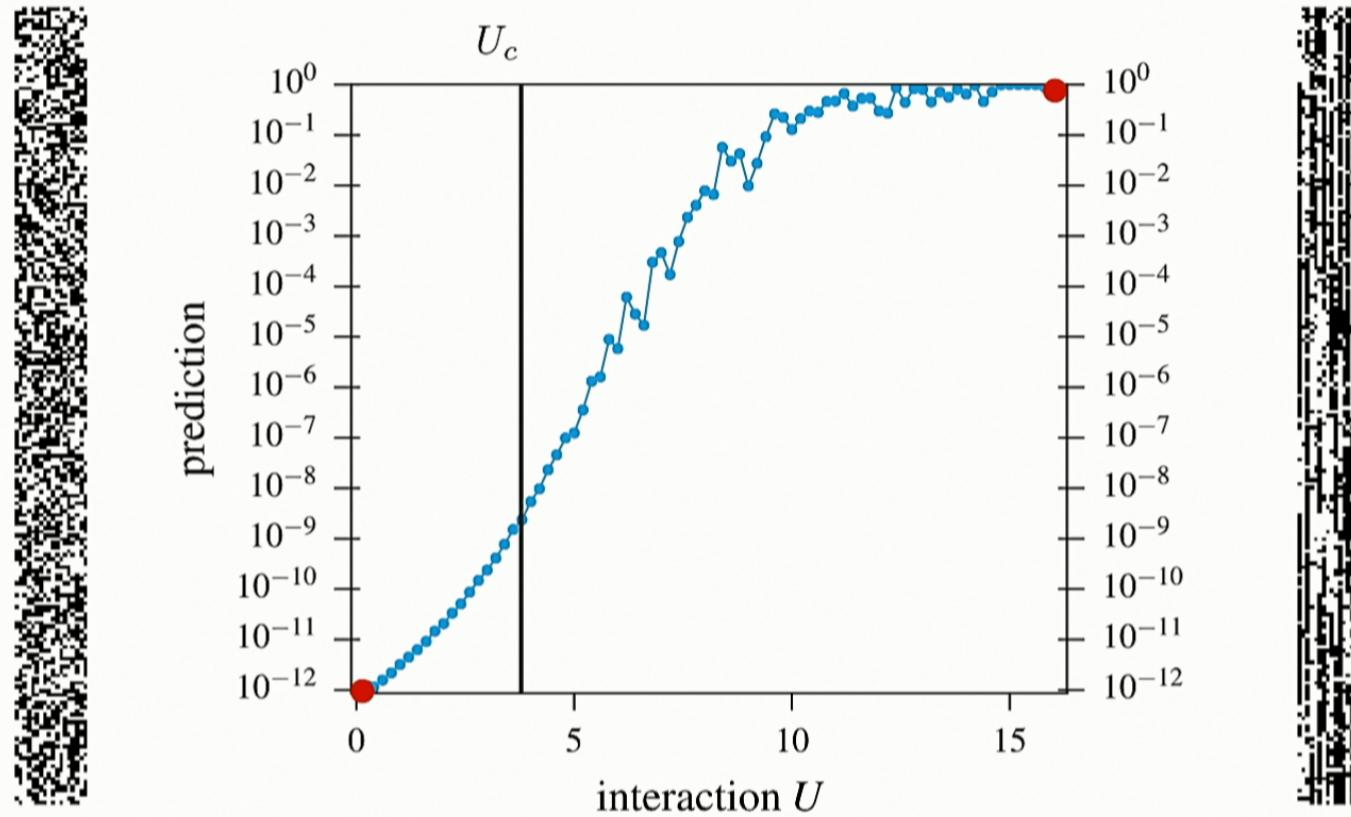
SM



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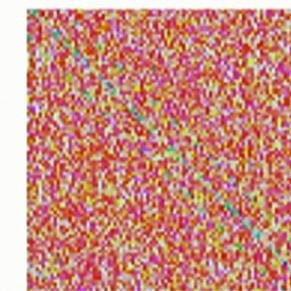
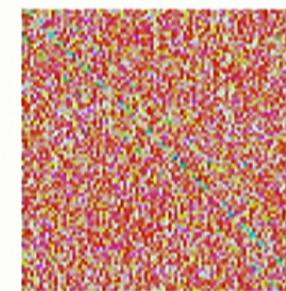
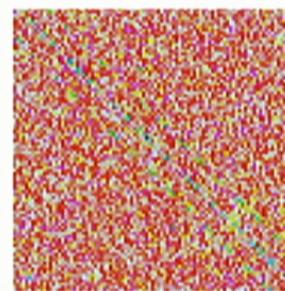
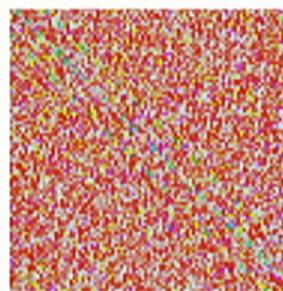
Supervised learning / auxiliary fields

coupling to magnetization

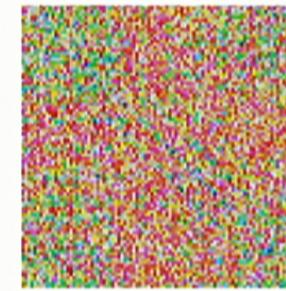
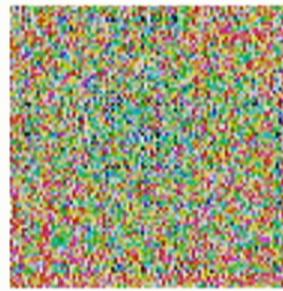


Supervised learning of Green's functions

Green's functions sampled as complex valued matrices
semi-metal

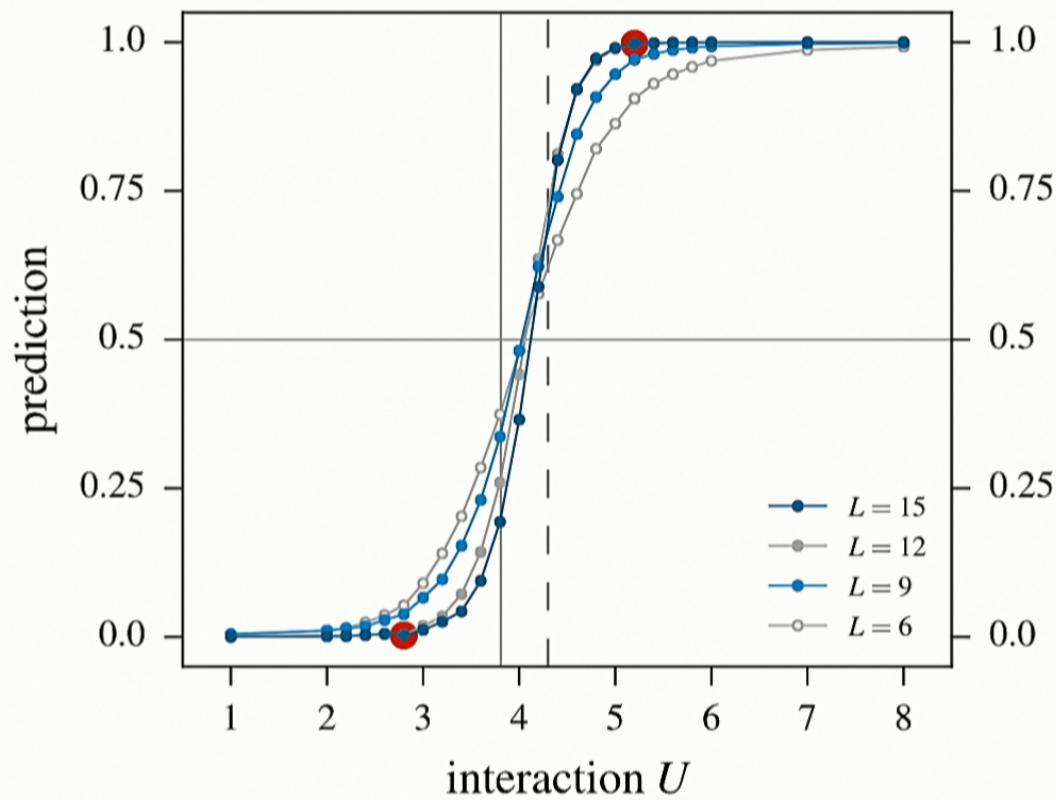


SDW



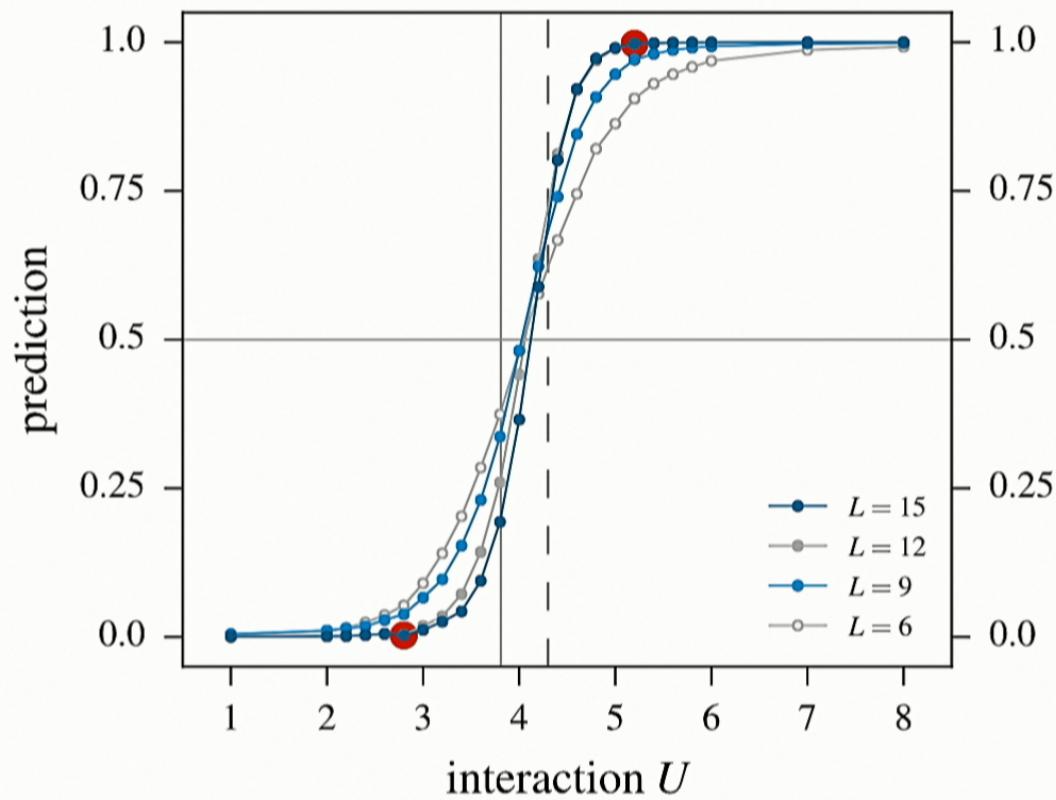
Spinful Fermions

Strong finite size effects close to transition [Nature 464 (7290), 847-851]
[Scientific Reports 2, 992]



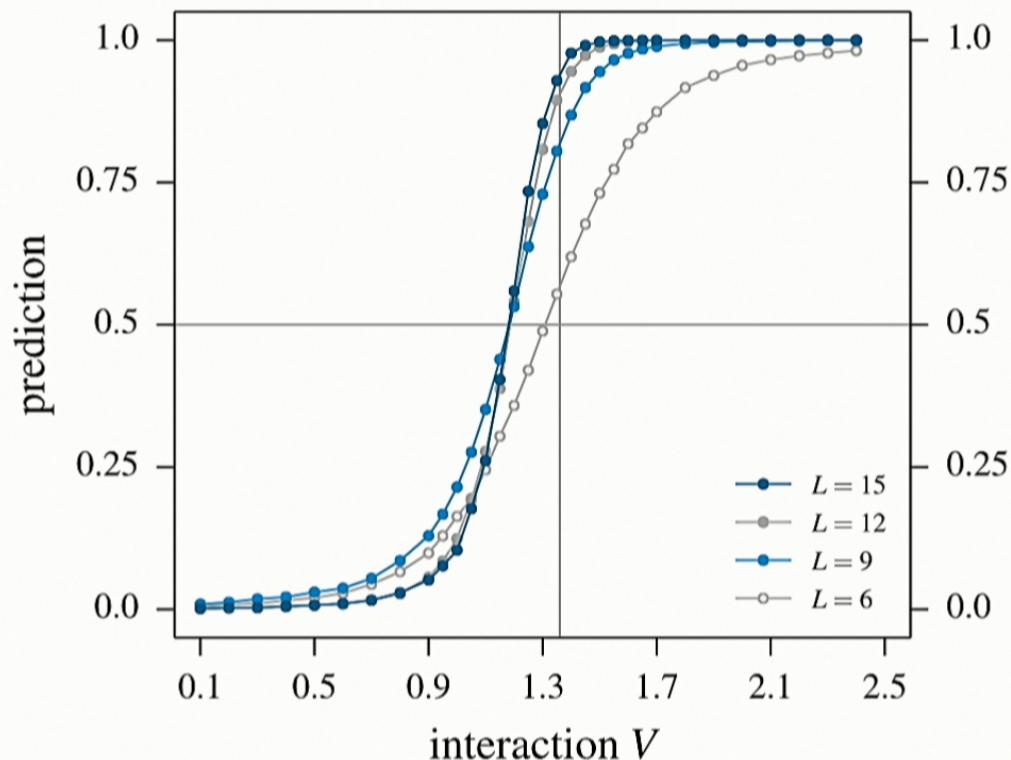
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Transfer Learning

Train **spinful** case - predict **spinless**
SDW and CDW are structurally similar



Conclusions

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

The ensemble of sampled [Green's functions](#) contains sufficient information to discriminate fermionic phases even in the presence of a severe sign problem.

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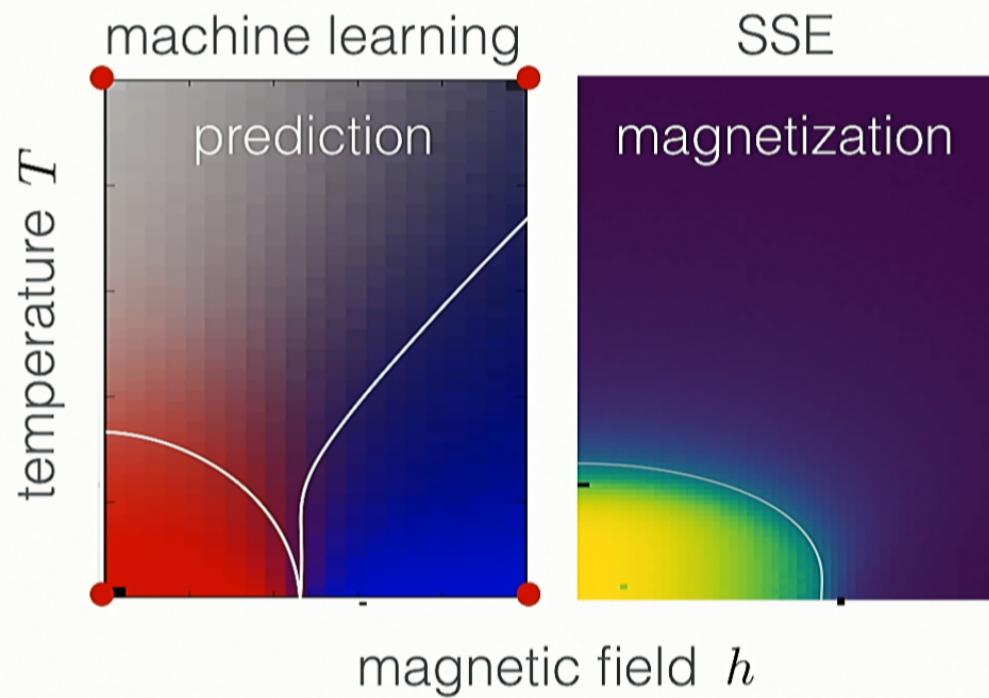
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Green's function based machine learning approach can be generalized to other quantum Monte Carlo flavors, e.g. the stochastic series expansion (SSE) techniques commonly applied to quantum magnets.

WORK IN PROGRESS

Transverse field Ising model

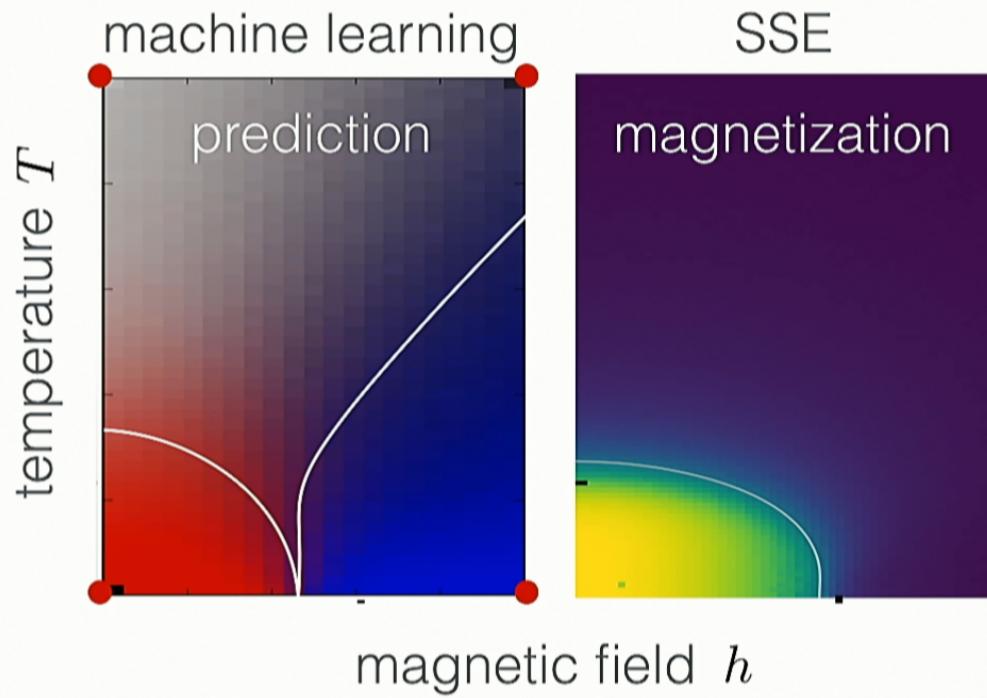
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Today's Discussion

4:00 pm, Bob room (4th floor)

Maria Schuld

Quantum Neural Networks

