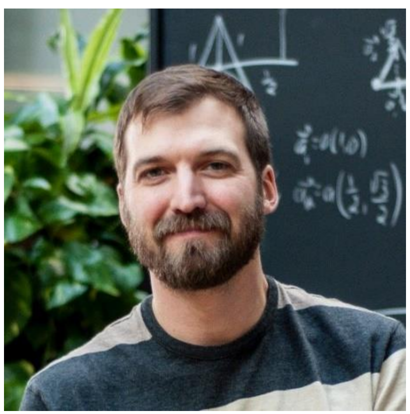
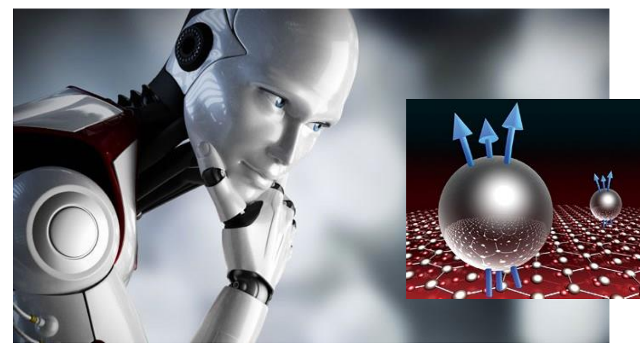
Quantum Loop Topography for Machine Learning

- on topological phases, phase transitions, and beyond

Yi Zhang
Cornell University





Roger G. Melko

Eun-Ah Kim

Cornell University

KITS workshop @ Beijing 2017

- Is machine learning quantum phases of matter:
  - Possible?
  - Reliable?
  - Necessary?

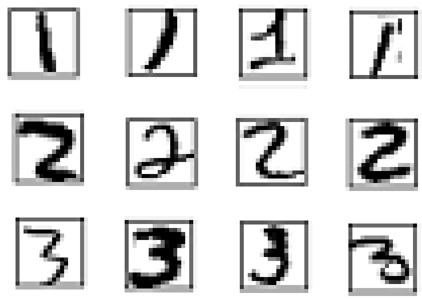
Neural network and machine learning

An image recognition problem

#1: …

#2: …

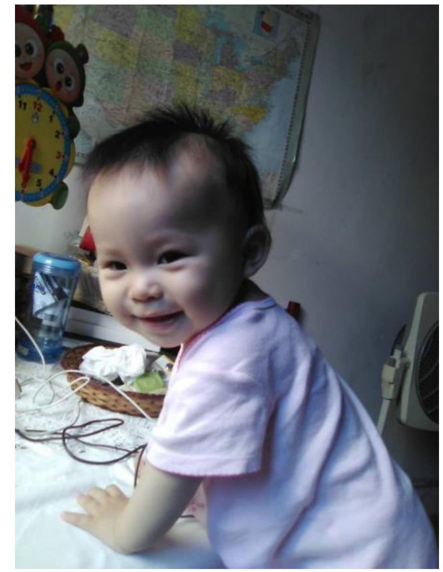
#3: …



…

Training set

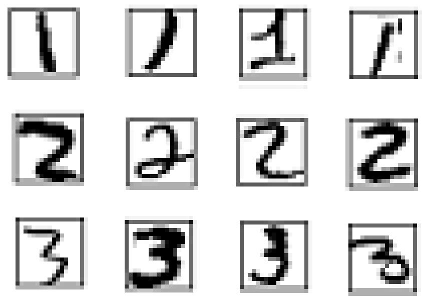
1. Child learning



An image recognition problem

504192

#1: …
#2: …
#3: …
…



Training set

1. Child learning

2. Application

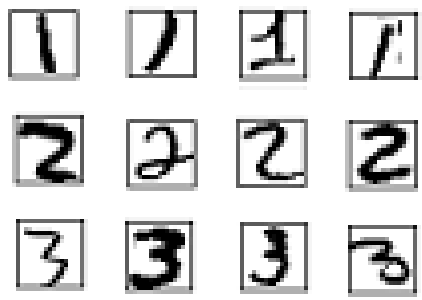
Neural network for image recognition

#1: …

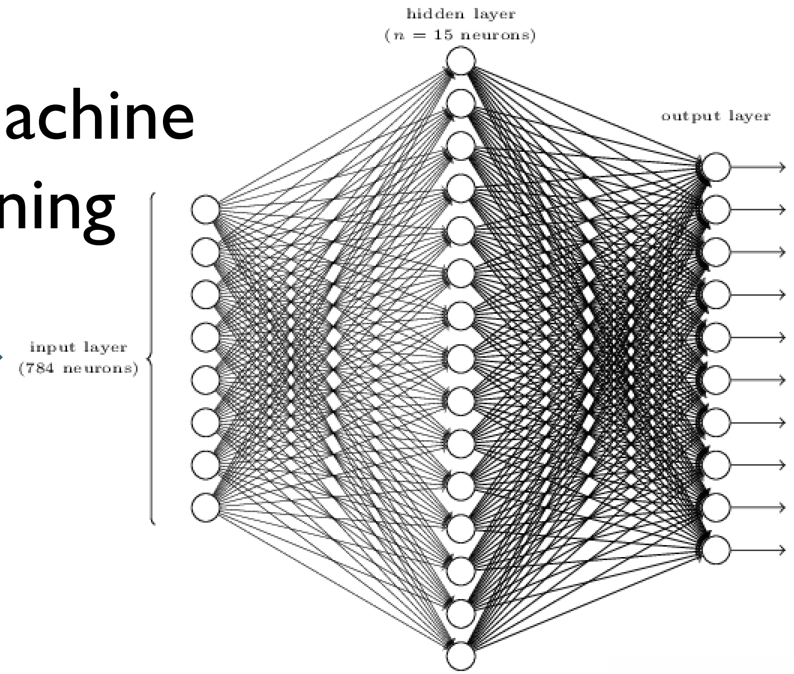
#2: …

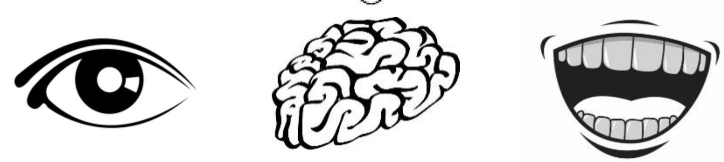
#3: …

…



1. Machine learning



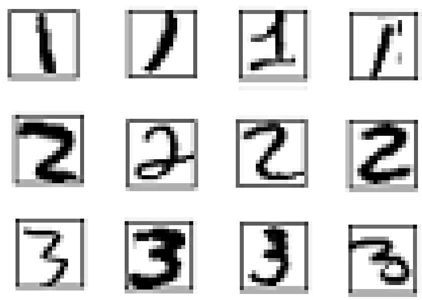


<u>Training set</u>

Online book: http://neuralnetworksanddeeplearning.com/

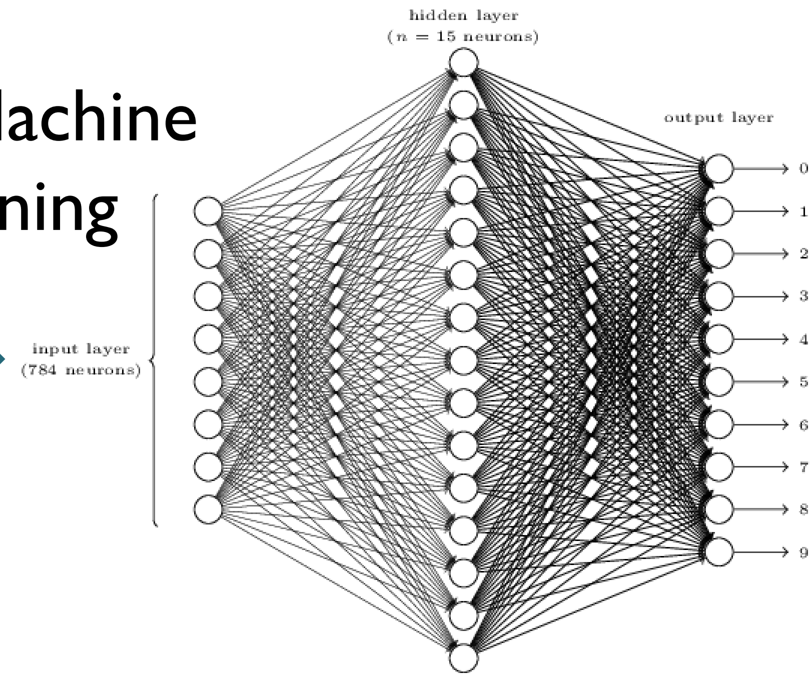
Neural network for image recognition

#1: ...
#2: ...
#3: ...
...



Training set

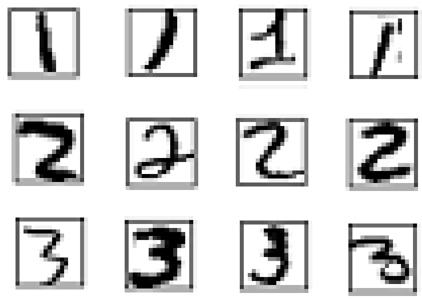
1. Machine learning



Optimal ***weights*** and ***biases***

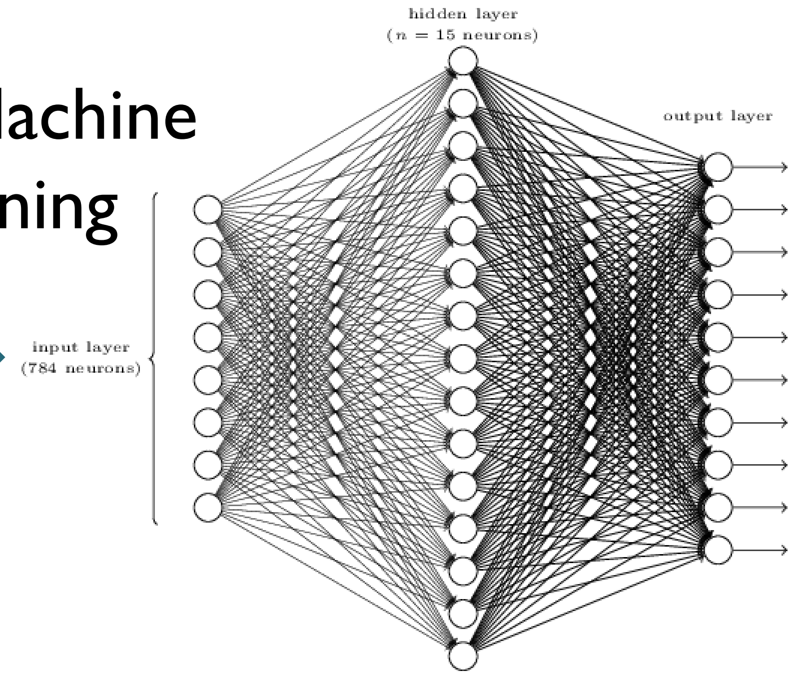
Online book: http://neuralnetworksanddeeplearning.com/

Neural network for image recognition

#1:  …
#2: …
#3: …
…

Training set

1. Machine learning



Optimal ***weights*** and ***biases***

2. Application

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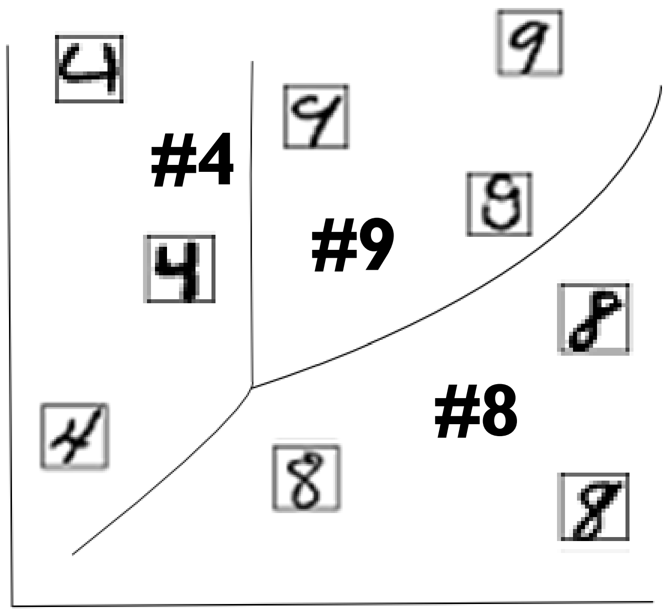
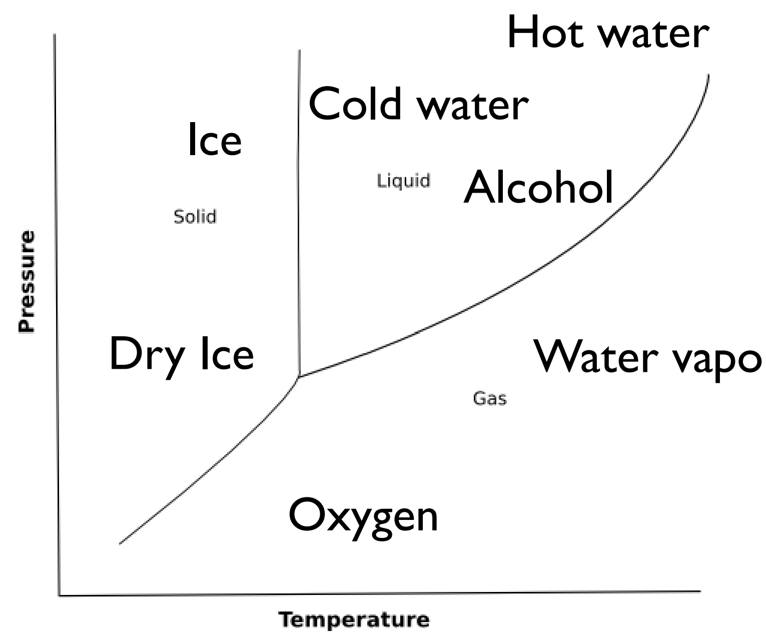
Neural network for image recognition

Online book: http://neuralnetworksanddeeplearning.com/

Machine learning as phase classification



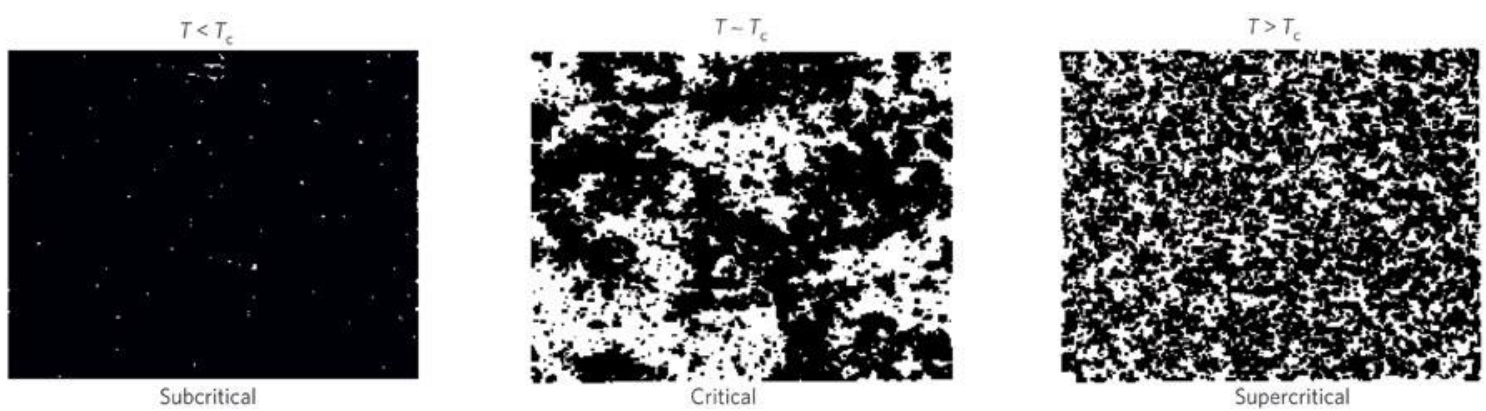


Machine learning in Condensed Matter Physics

- **Machine learning phases of matter and phase transitions (for phase diagrams)**
- Restricted Boltzmann Machines, tensor networks, and neural network states
- Algorithmic development
- Material and molecule simulations
- Renormalization group
- Many more …

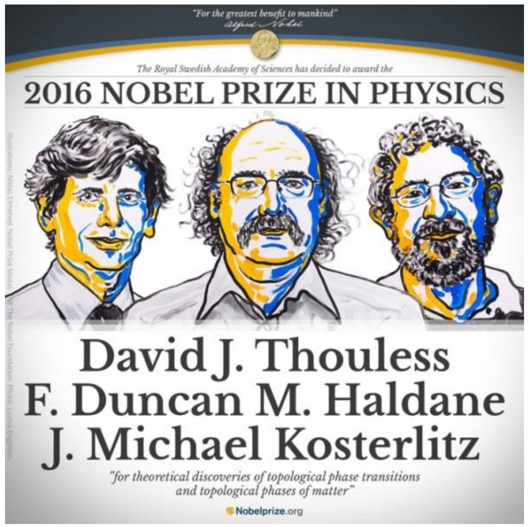
Machine learning in Condensed Matter Physics

- **Machine learning phases of matter and phase transitions (for phase diagrams)**
  - *J. Carrasquilla and R. G. Melko (2016)*
  - *L. Wang (2016)*
  - *E.P.L. van Nieuwenburg, Y.-H. Liu, and S.D. Huber (2016)*
  - *P. Broecker, J. Carrasquilla, R. G. Melko, and S. Trebst (2016)*
  - *K. Ch'ng, J. Carrasquilla, R. G. Melko, and E. Khatami (2016)*
  - *T. Ohtsuki and T. Ohtsuki (2016)*
  - *And more …*



Online book: http://neuralnetworksanddeeplearning.com/

Machine learning phases of matter



- 1. quantum and sometimes strongly correlated
- 2. lack of order parameter and computationally difficult
- 3. discrete characterization of topological indices
- 4. brute force machine learning doesn't work

- Is machine learning ***topological*** phases of matter:
  - Possible? Reliable? Necessary?

Selected for a Viewpoint in *Physics*
PRL **118,** 216401 (2017) PHYSICAL REVIEW LETTERS week ending 26 MAY 2017

Quantum Loop Topography for Machine Learning

Yi Zhang[*] and Eun-Ah Kim[†]
Department of Physics, Cornell University, Ithaca, New York 14853, USA

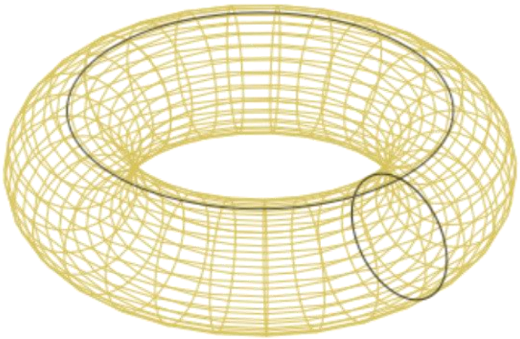
Methods for topological phases of matter

- Checking whether a model hosts a strongly-correlated topological order:
  - Ground-state degeneracy on nontrivial manifolds
  - Topological entanglement entropy
  - Minimum entropy states
  - …

faces harsh constraints and cost.

Methods for topological phases of matter

- Minimum entropy states
  - Constraints
    - All degenerate ground states
    - Nontrivial manifold
  - Cost



YZ, Tarun Grover, Ari Turner, Masaki Oshikawa, and Ashvin Vishwanath (2012).

Methods for topological phases of matter

- Minimum entropy states
  - Constraints
    - All degenerate ground states
    - Nontrivial manifold
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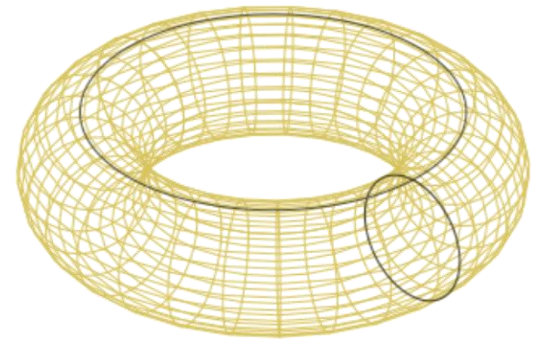


Entanglement entropy $S = -\log\langle Swap\rangle$ → Differences between several S for TEE γ → Various trials for maxima of γ → Various points in the phase diagram

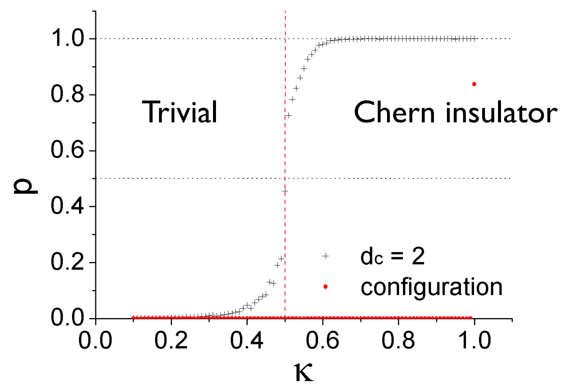
Parallel MC computation:

$$\frac{10^5\text{CPUmins} \times 100 \times 100}{256\text{CPUs}}$$

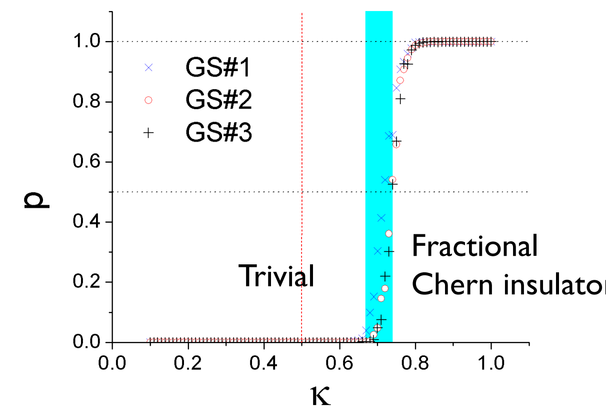
$= \underline{\textbf{\textit{7.5 years}}}\ldots$

YZ, Tarun Grover, Ari Turner, Masaki Oshikawa, and Ashvin Vishwanath (2012).

Calculations take days, if not years

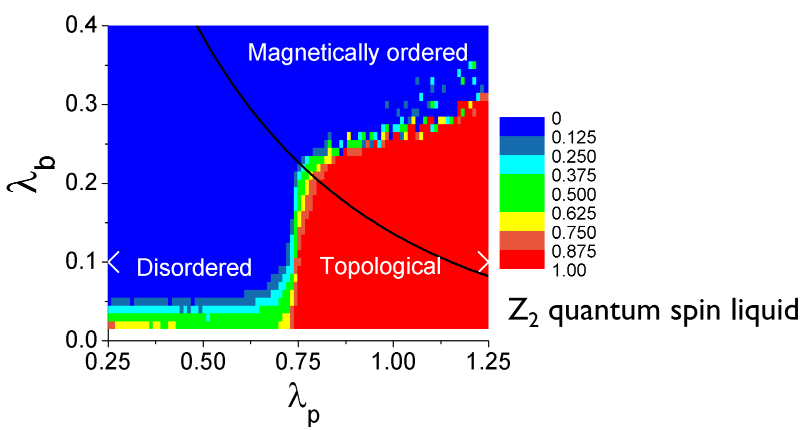


YZ, Eun-Ah Kim(2016)

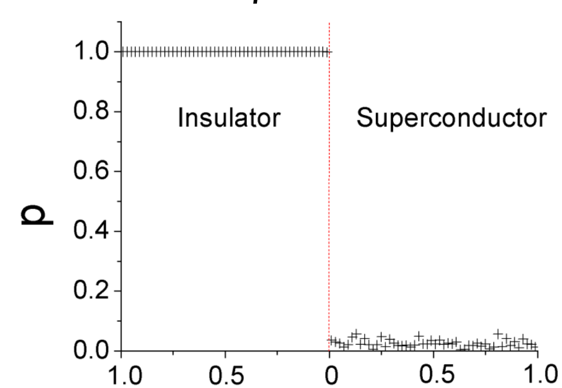


YZ, Eun-Ah Kim(2016)

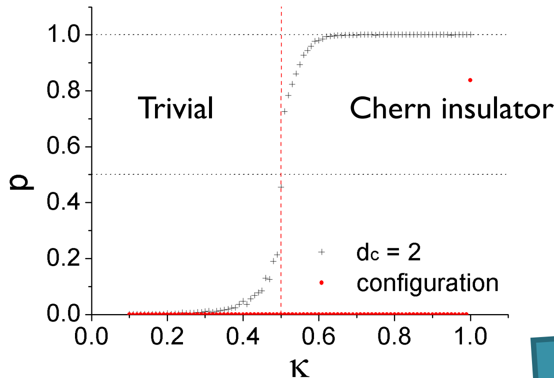
YZ, R. G. Melko, Eun-Ah Kim(2017)



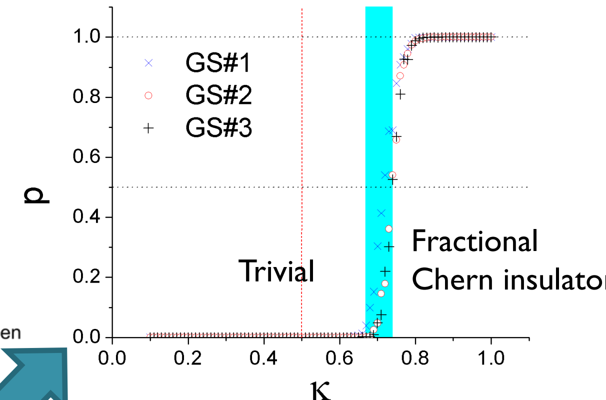
Unpublished data



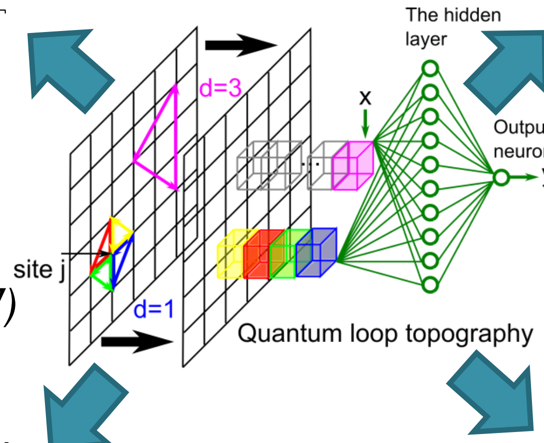
Not years, not days, just ***minutes***



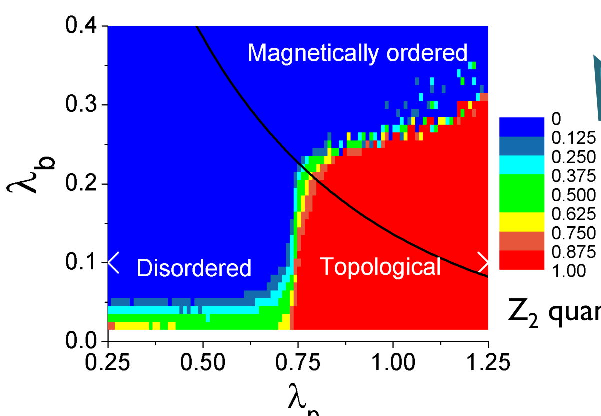
YZ, Eun-Ah Kim(2016)



YZ, Eun-Ah Kim(2016)

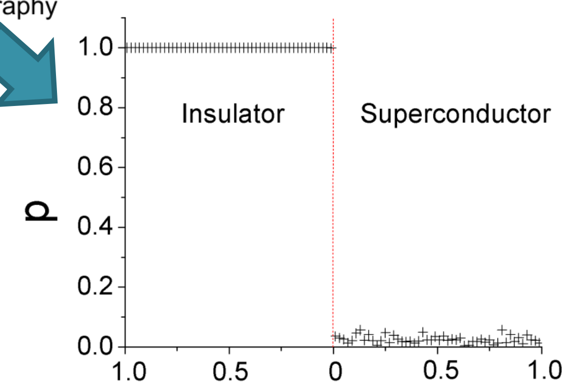


YZ, R. G. Melko, Eun-Ah Kim(2017)



Z_2 quantum spin liquid

Unpublished data



How was it done?

What is Quantum Loop Topography?

Selected for a Viewpoint in *Physics*

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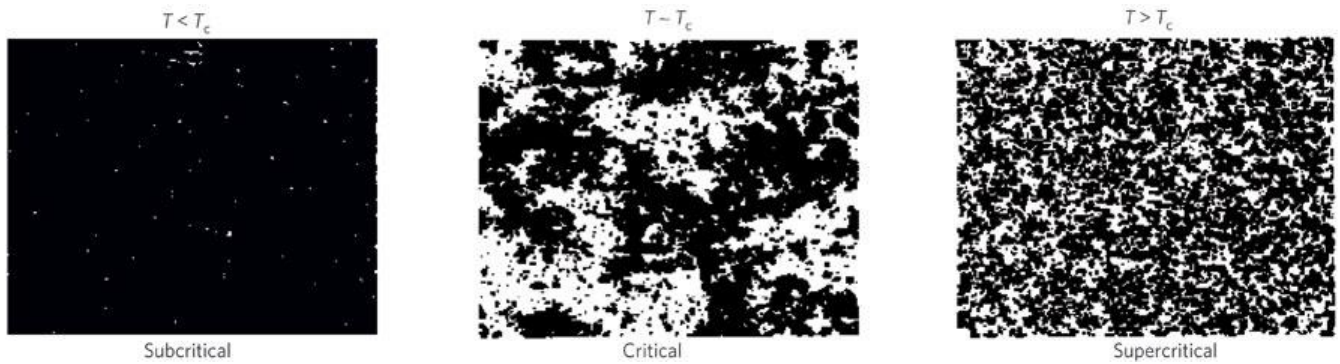
Quantum Loop Topography for Machine Learning

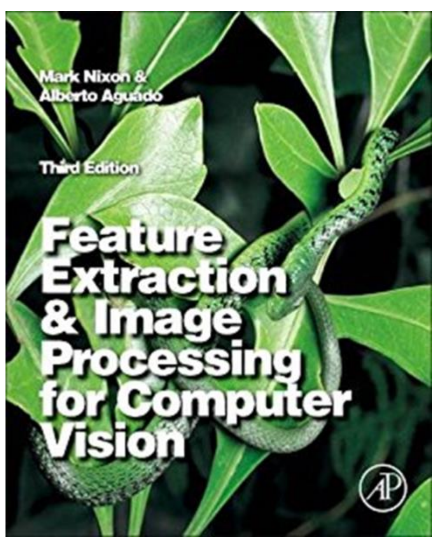
Yi Zhang[*] and Eun-Ah Kim[†]

Department of Physics, Cornell University, Ithaca, New York 14853, USA

Feature selection in machine learning

* Order parameter as feature:





I. Guyon and A. Elisseeff, J. Mach. Learn. Res.3, 1157 (2003)

Feature selection in machine learning

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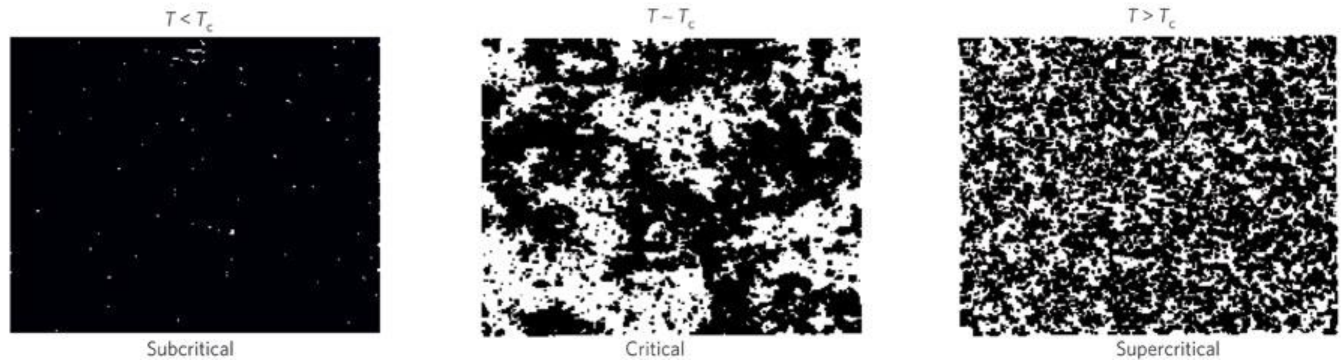
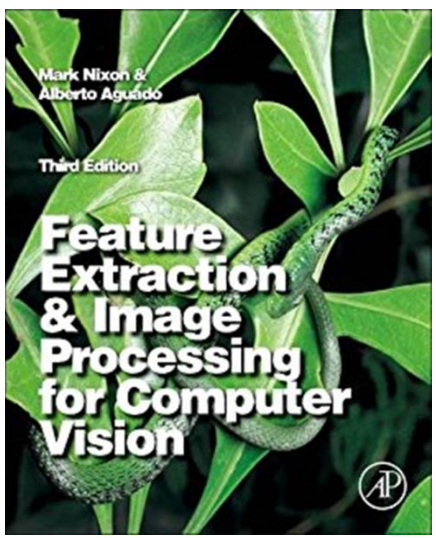
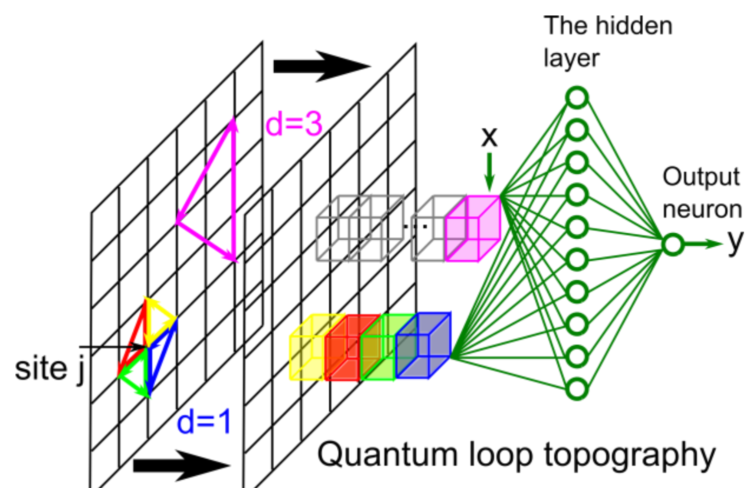




* Essential operators as feature:



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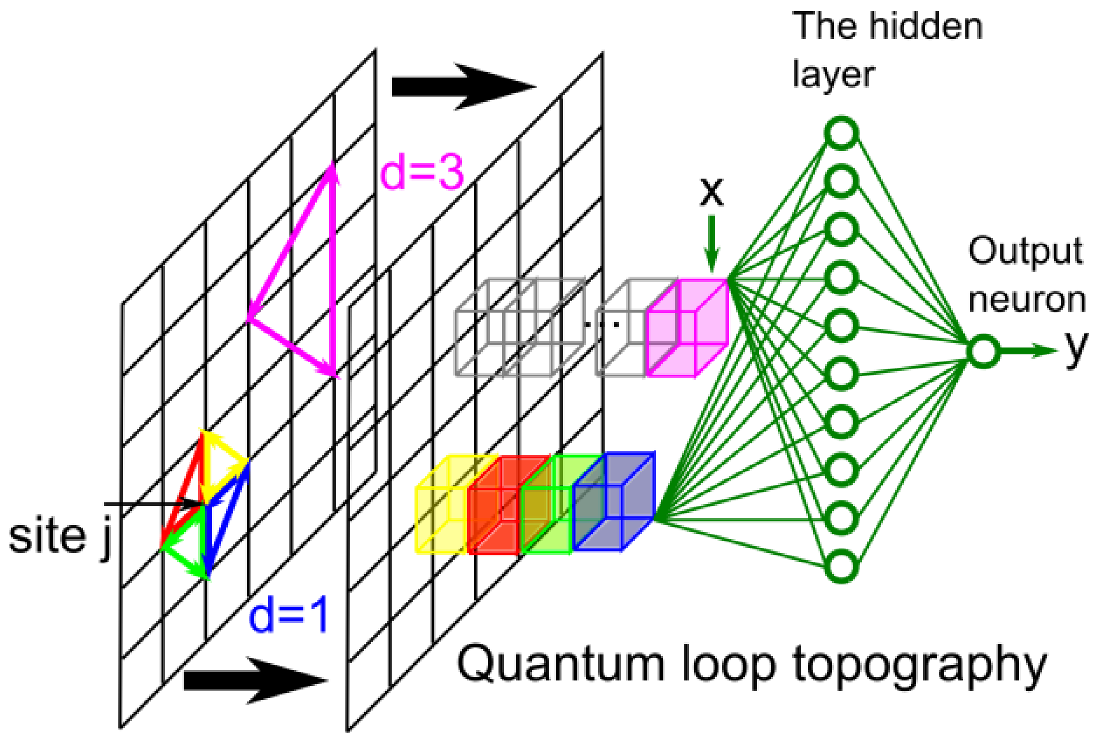
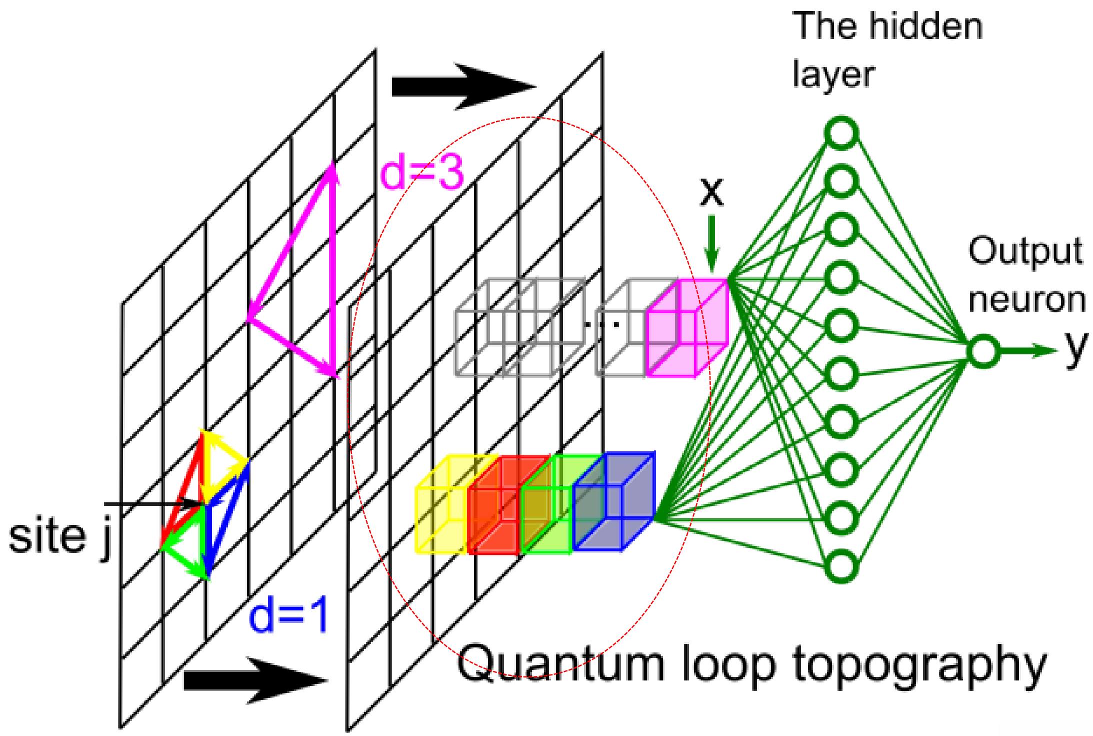
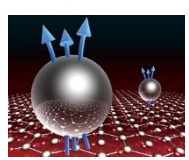
What is Quantum Loop Topography?



- Left side: ***input lattice model***
- Mid-right: simple, fully-connected ***neural network***
- Right side: ***output*** judgement on the corresponding phase

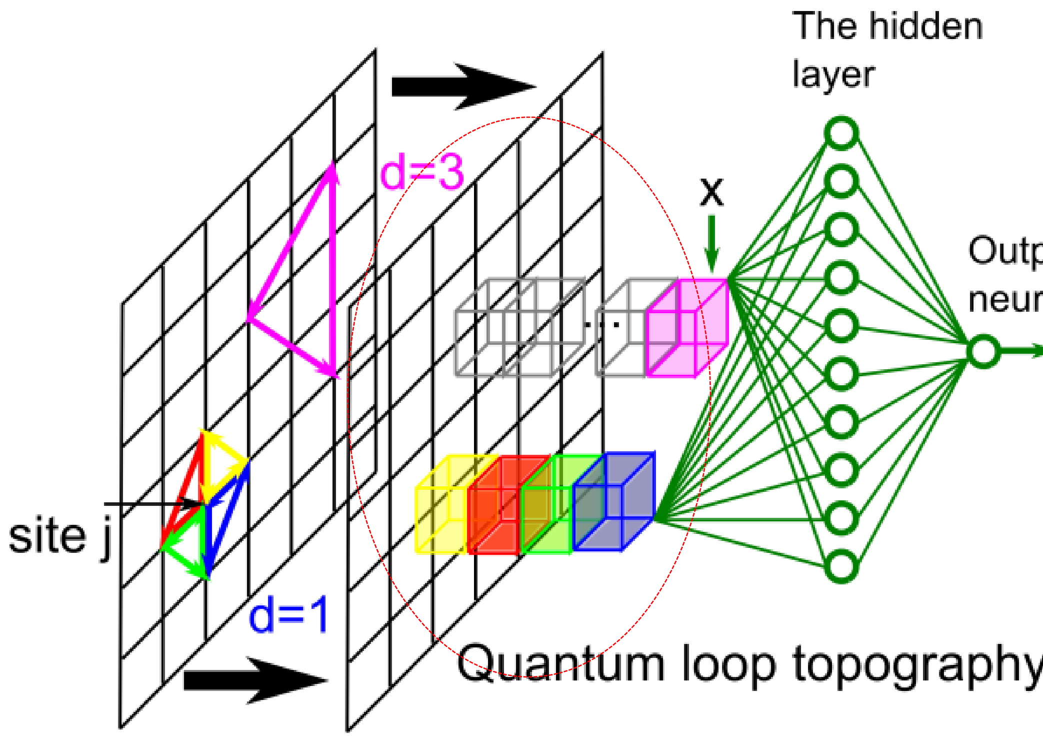
What is Quantum Loop Topography?





many-body state – ? – classical image

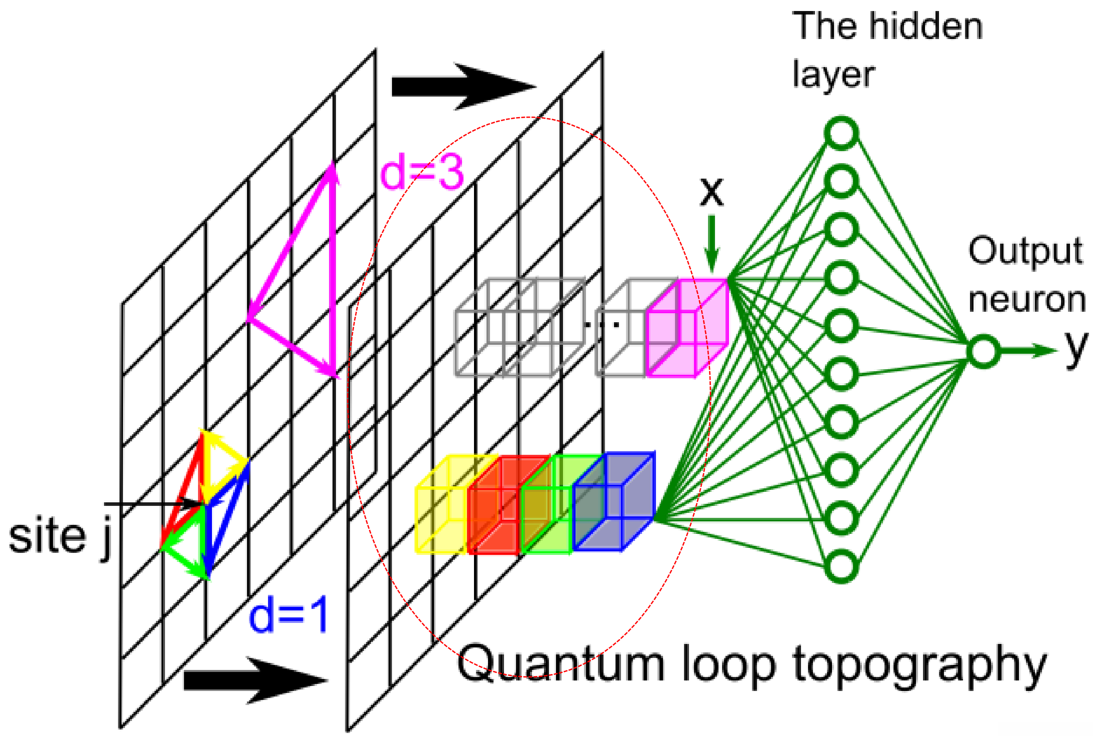
What is Quantum Loop Topography?



- Mid-left: ***quantum loop topography***

many-body state – quantum operators – classical image

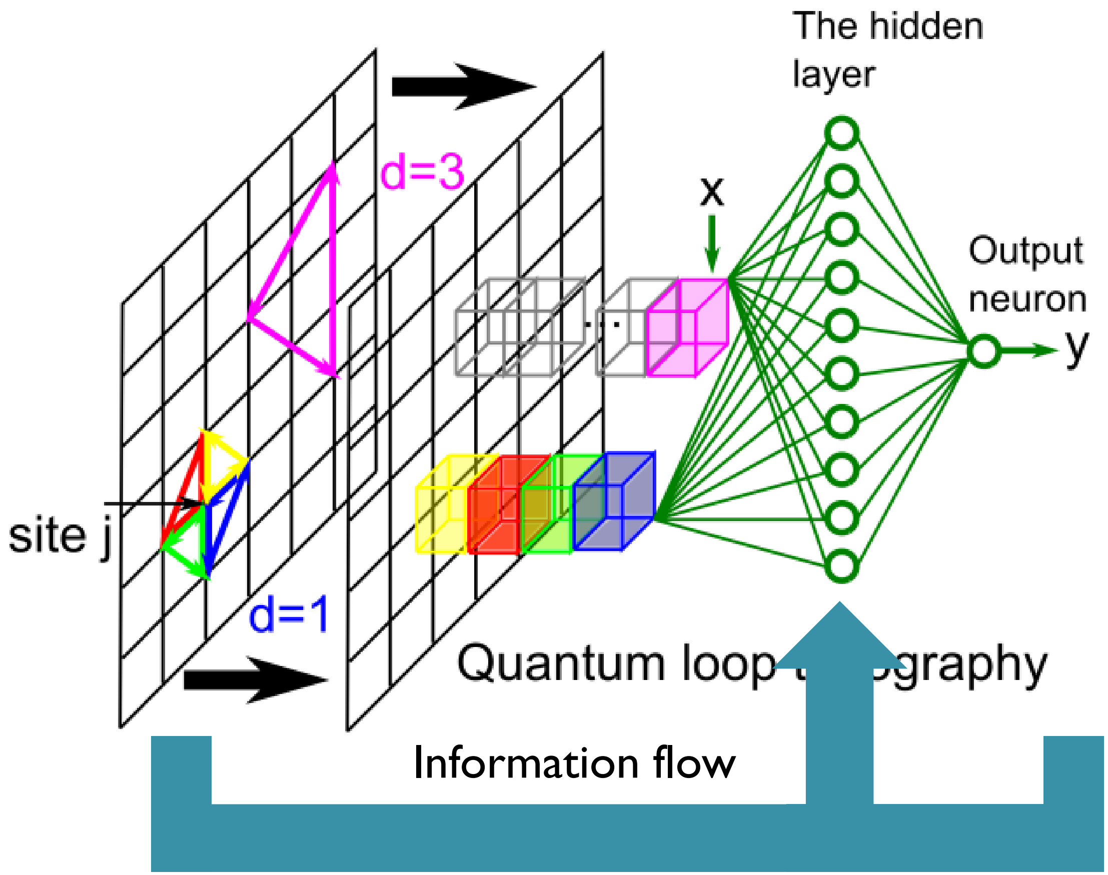
What is Quantum Loop Topography?



- Mid-left: ***quantum loop topography***

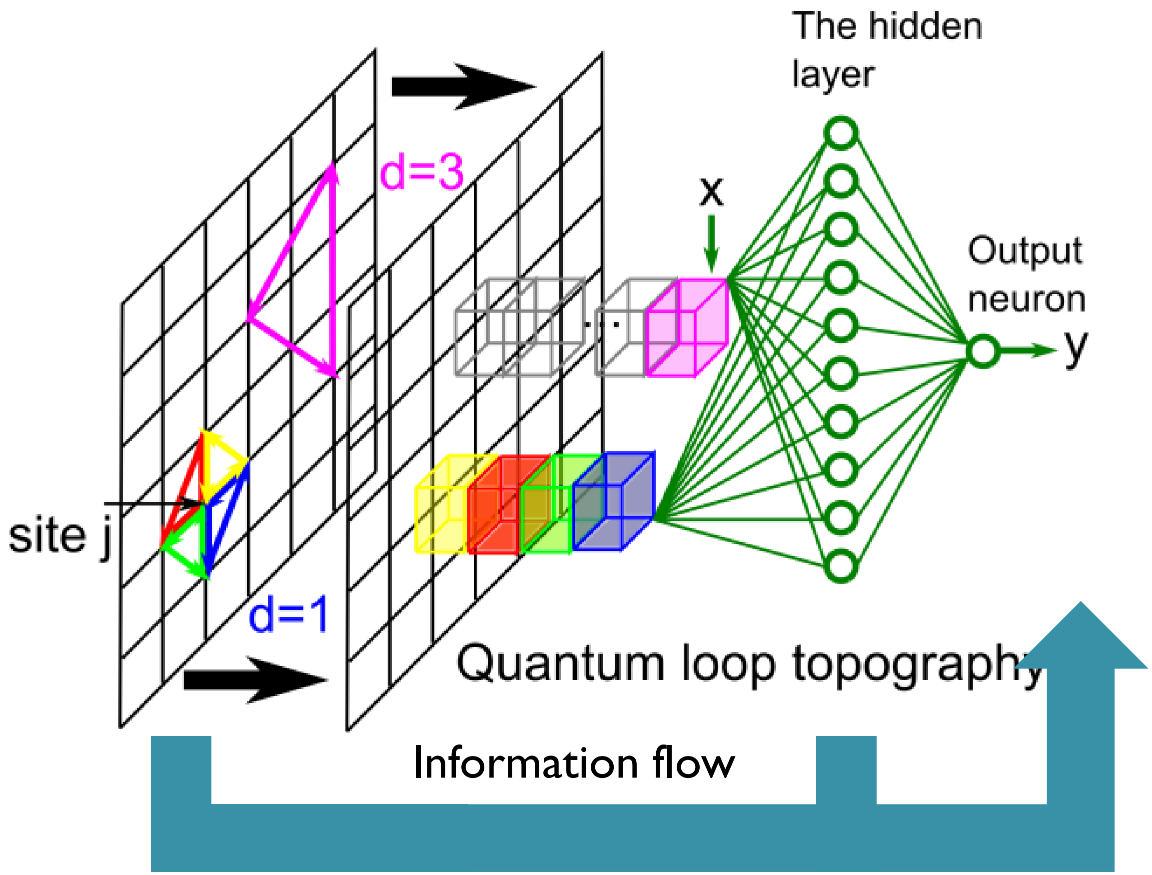
  ensemble of operators that contain relevant information

What is Quantum Loop Topography?



- ***Training***: using examples to ***optimize*** the neural network

What is Quantum Loop Topography?

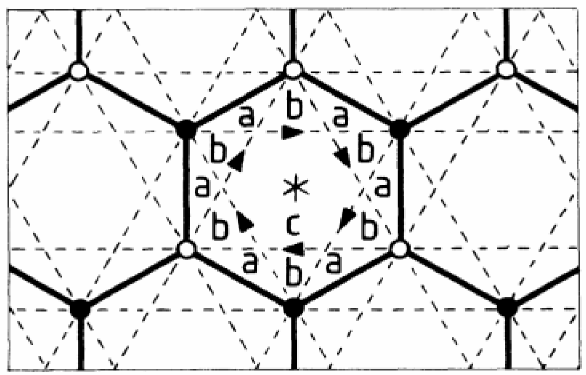


- ***Testing***: using the optimized neural network to ***identify***

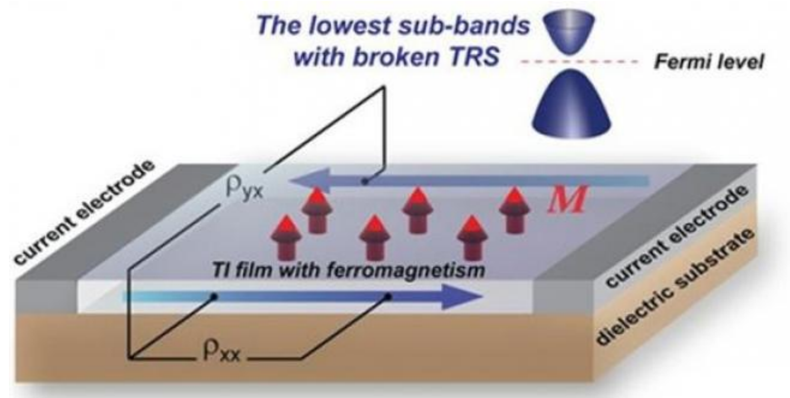
Examples: machine learning topological phases with ***quantum loop topography***

Chern Insulator

- Also known as quantum anomalous Hall state



F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).



Cui-Zu Chang, Jinsong Zhang, Xiao Feng, Jie Shen, et al., Science 340, 167 (2013).

- Non-interacting topological phase
- Similar to the Integer quantum Hall state, but
  - On a lattice
  - Without external magnetic field

Hall conductivity revisited

- As a physical response, Hall conductivity is ***characteristic*** for the quantum Hall phases.
  - Topological index
  - Quantized and protected

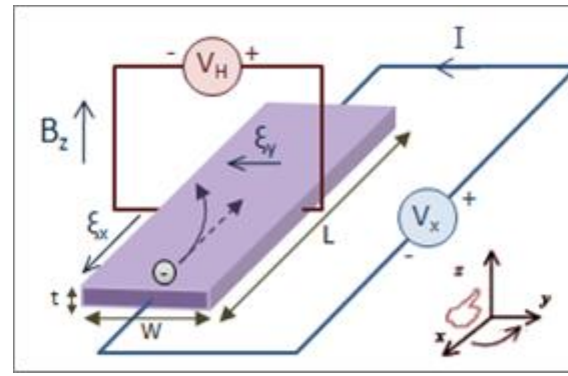


Image source: Quora

Hall conductivity revisited

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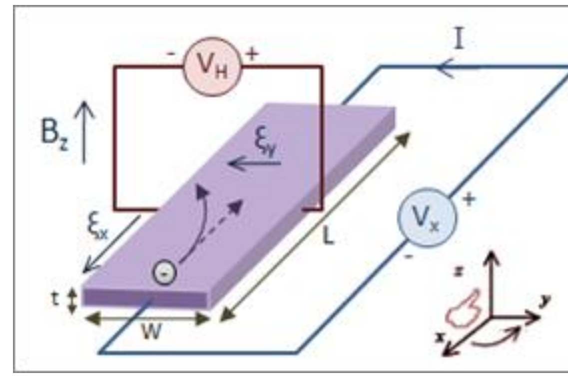
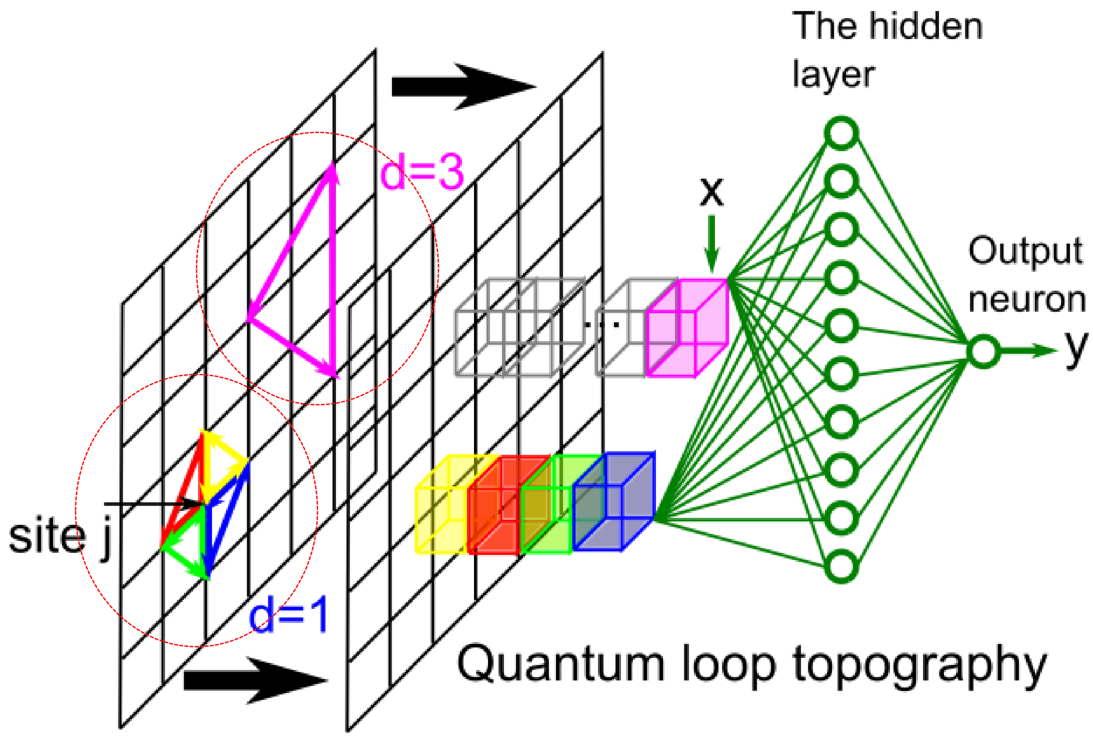


- Hall conductivity of a non-interacting fermionic systems:

$$\sigma_{xy} = \frac{e^2}{h} \cdot \frac{1}{N} \sum 4\pi i P_{jk} P_{kl} P_{lj} S_{\triangle jkl} \quad P_{ij} \equiv \langle c_i^\dagger c_j \rangle$$

A. Kitaev (2006);YZ, Eun-Ah Kim (2016)

Quantum Loop Topography for Chern Insulator



- ***Quantum loop topography***: samples of two-point operators that form (triangle) loops ijk $\boxed{\tilde{P}_{jk}\tilde{P}_{kl}\tilde{P}_{lj}}$

Operator are evaluated at Monte Carlo step α: $\tilde{P}_{jk} \equiv \left\langle c_j^\dagger c_k \right\rangle_\alpha$

YZ, Eun-Ah Kim (2016)

Machine learning and Monte Carlo

- Expectation value in Monte Carlo calculations converges as ~ n(-1/2)

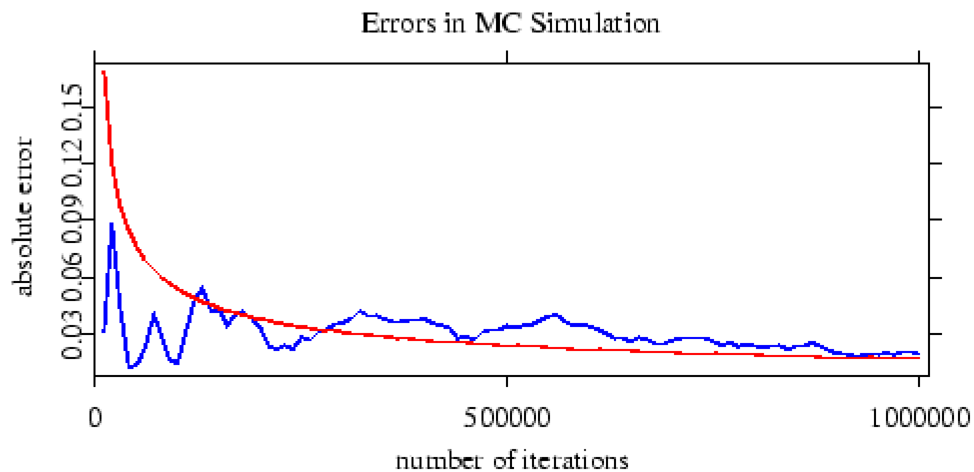


Image source: research data center

Machine learning and Monte Carlo

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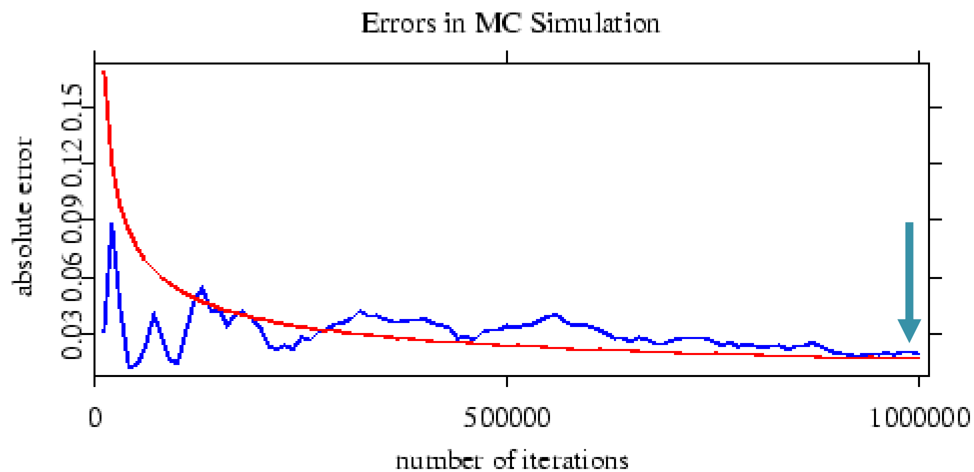

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Machine learning and Monte Carlo

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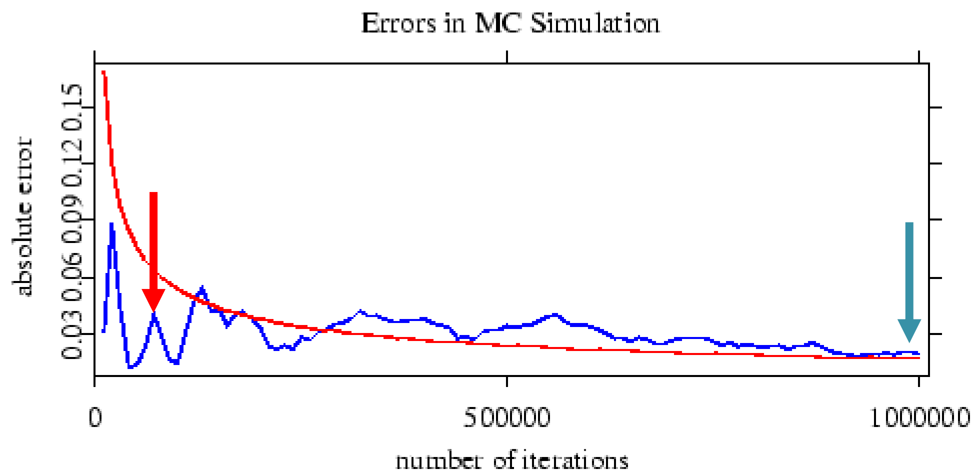
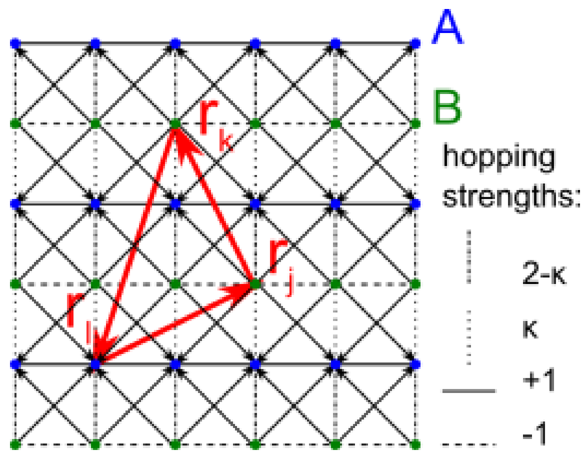
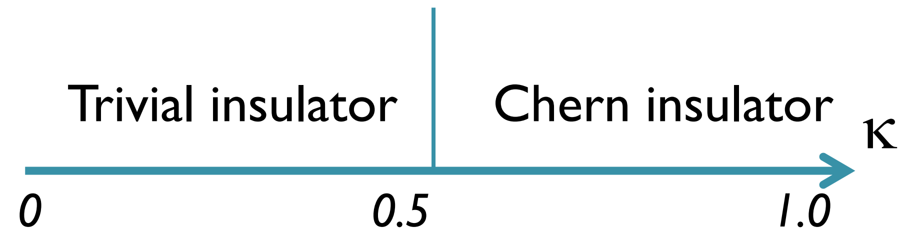


Image source: research data center

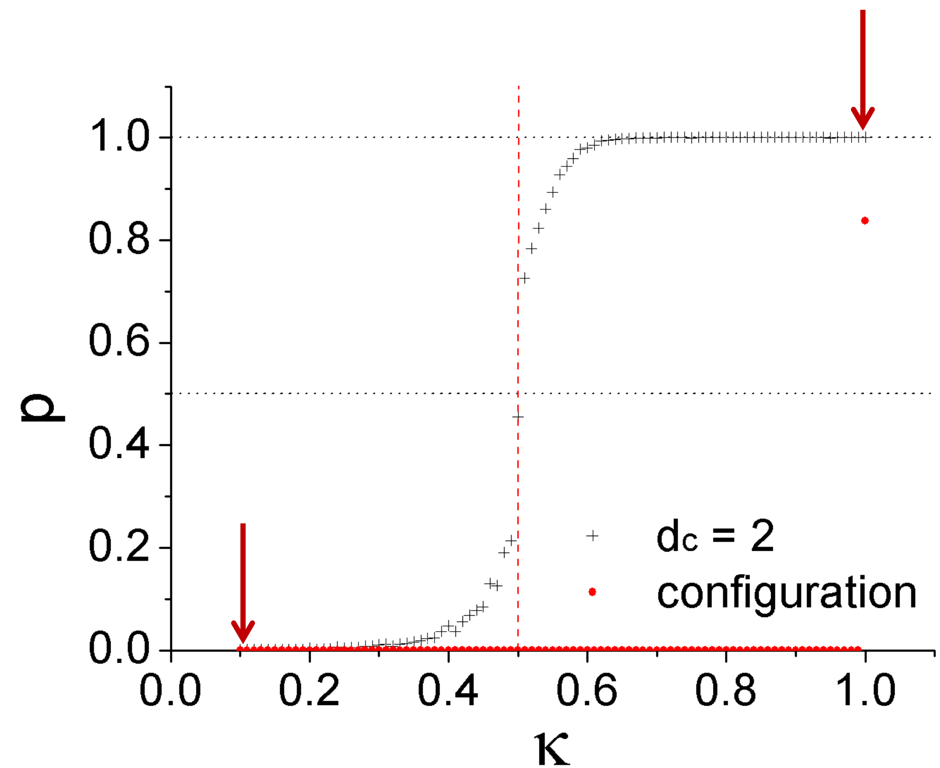
Machine learning Chern Insulator





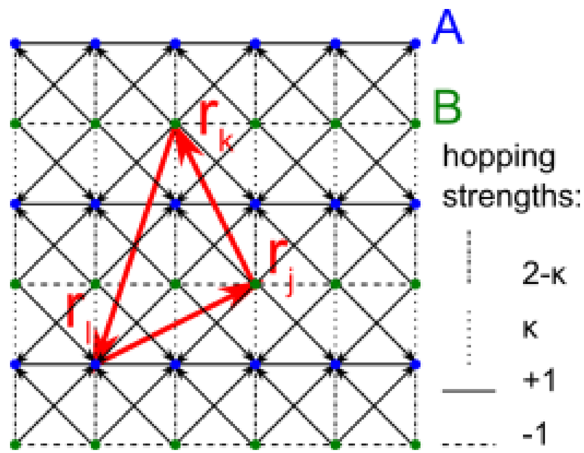
- Training set

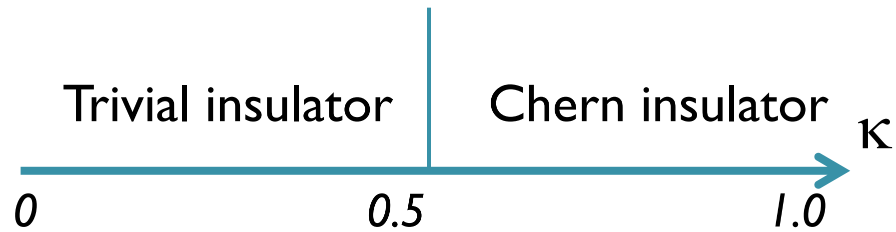
Trivial	κ=0.1
Topological	κ=1.0



YZ, Eun-Ah Kim (2016)

Machine learning Chern Insulator





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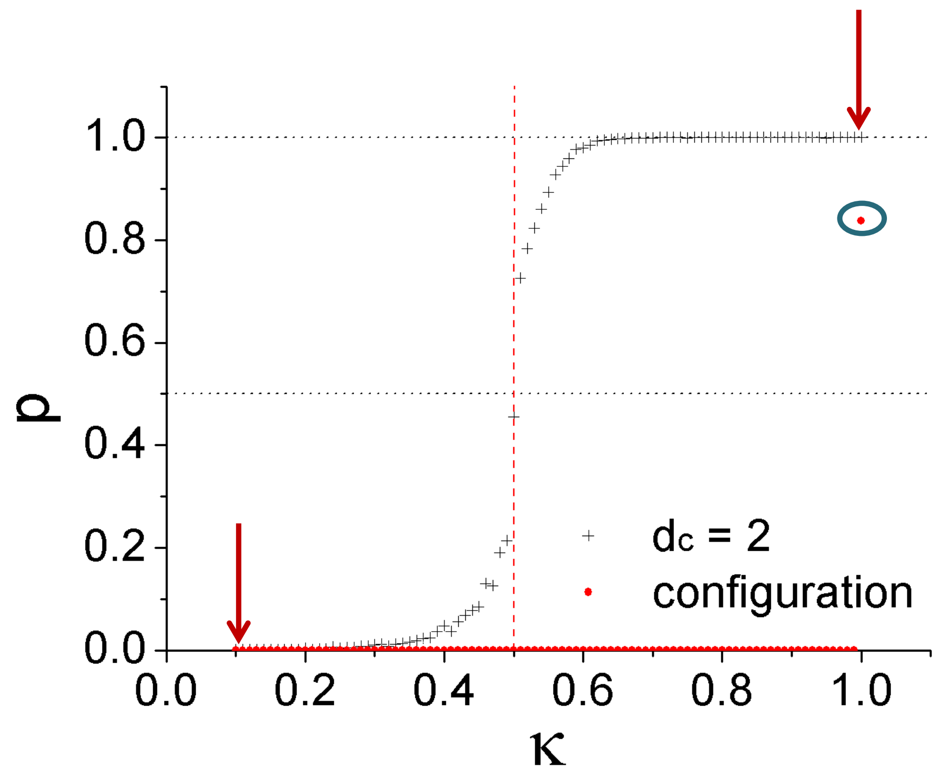
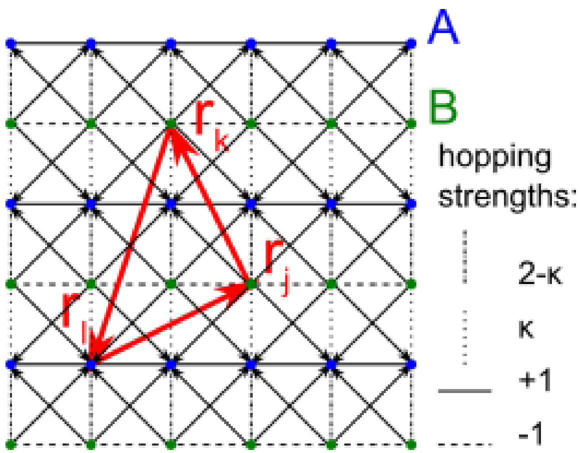
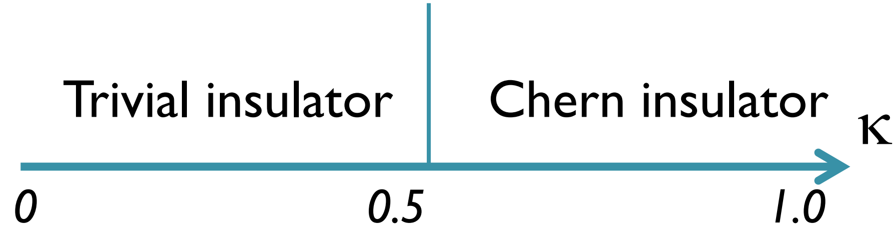


YZ, Eun-Ah Kim (2016)

Machine learning Chern Insulator

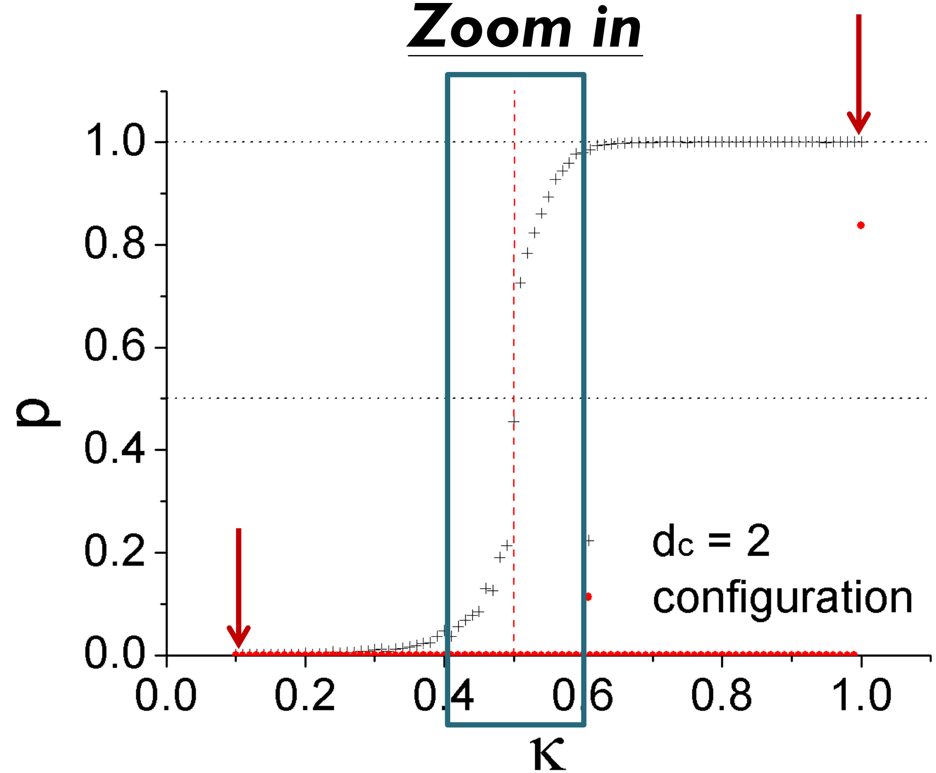




- Training set

Trivial	κ=0.1
Topological	κ=1.0

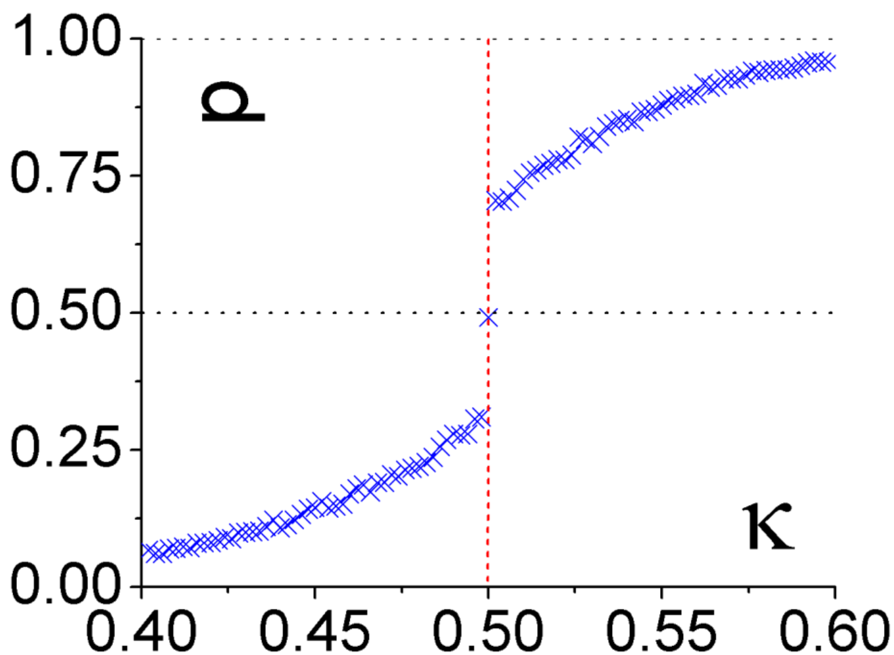
Zoom in



YZ, Eun-Ah Kim (2016)

Machine learning Chern Insulator

- Phase transitions: ***non-analyticity*** at the critical point



YZ, Eun-Ah Kim (2016)

ν=1/3 Fractional Chern Insulator

- ν=1/3 fractional Chern insulator (FCI)
  - A ***strongly-correlated*** topological order
  - Degenerate ground states on a torus via b.c.
  - Candidate variational wave functions

$$\Psi_{1/3}(r_1, r_2 \ldots, r_N) = \Phi^3(r_1, \ldots, r_N)$$

$\Phi(r_1, \ldots, r_N)$ is the wave function of a Chern insulator.

- $$\begin{tikzcd} \text{GS\#1} \arrow[r, "\textit{Flux}"] & \text{GS\#2} \arrow[r, "\textit{Flux}"] & \text{GS\#3} \arrow[ll, bend left, "\textit{Flux}"] \end{tikzcd}$$

YZ, Tarun Grover, Ashvin Vishwanath (2011)

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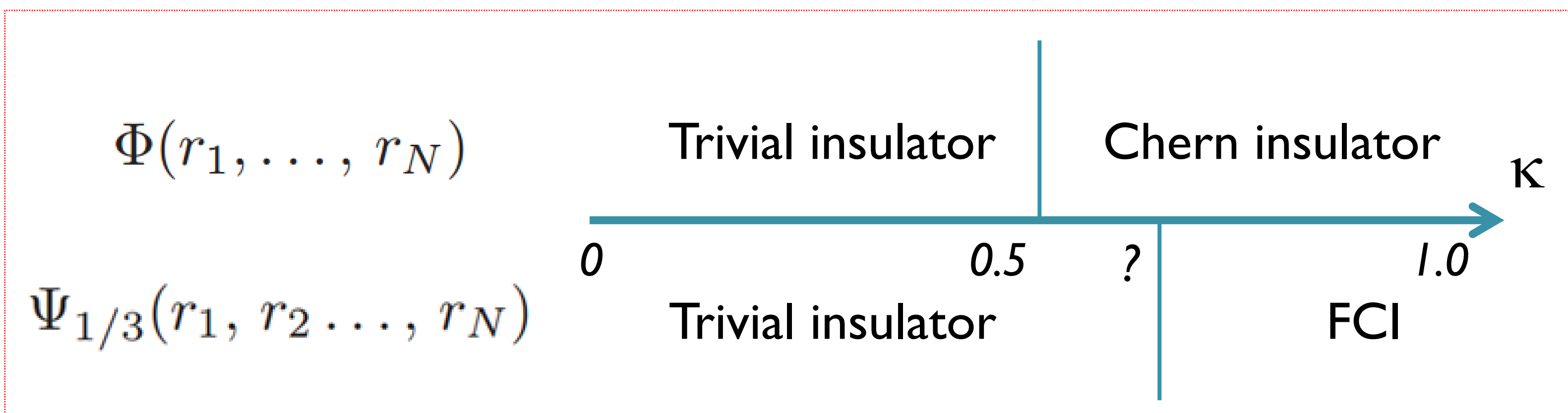
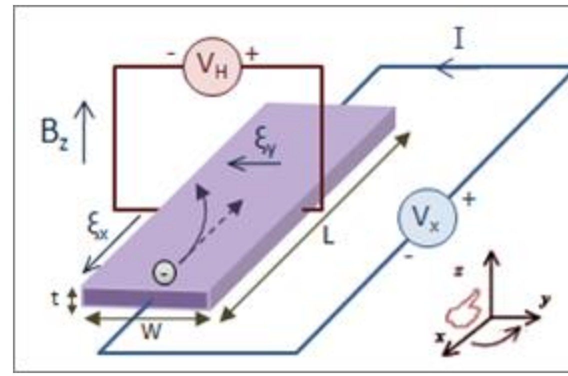


YZ, Tarun Grover, Ashvin Vishwanath (2011)

Machine learning Fractional Chern Insulator

- As a physical response, Hall conductivity is ***characteristic*** for the quantum Hall phases.
  - Topological index
  - Quantized and protected



- Hall conductivity of an interacting fractional system?

$$\cancel{\sigma_{xy} = \frac{e^2}{h} \cdot \frac{1}{N} \sum 4\pi i P_{jk} P_{kl} P_{lj} S_{\triangle jkl}} \quad P_{ij} \equiv \langle c_i^\dagger c_j \rangle$$

$$\sigma_{xy} = \frac{e^2}{h} \cdot \frac{1}{N} \sum 4\pi i \left(P_{jk} P_{kl} P_{lj} \right)^{?} \mathrm{X}\, ?$$

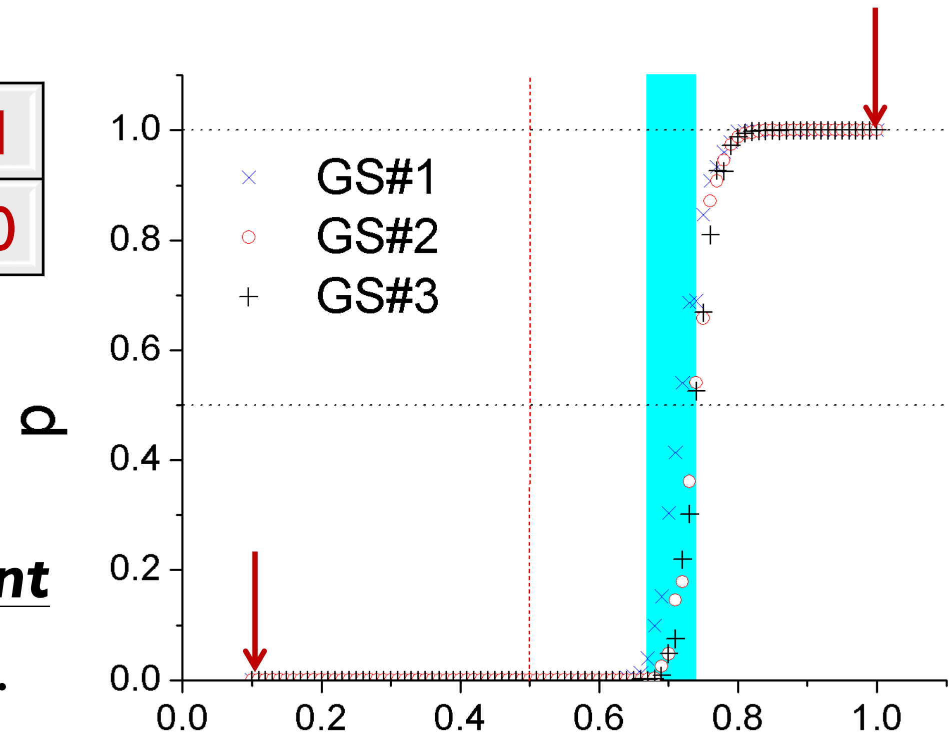
Machine learning Fractional Chern Insulator

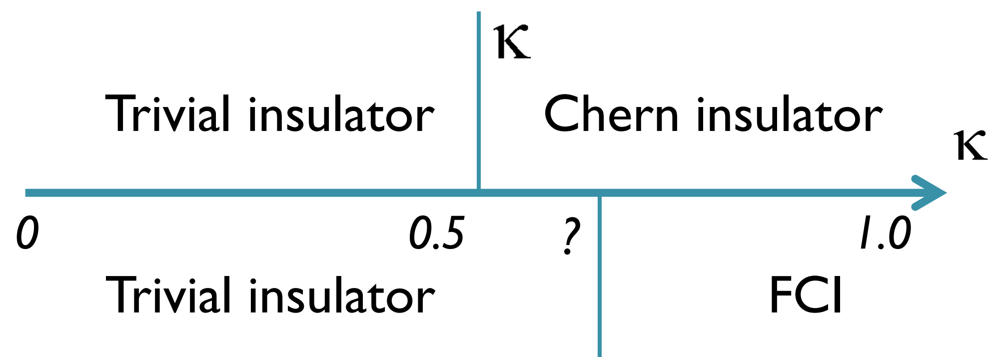
- Training group

Trivial	$\kappa=0.1$
Topological*	$\kappa=1.0$

*: ***GS#1 only***.

- $\kappa_c \sim 0.7$ is ***consistent*** with our benchmark.





YZ, Eun-Ah Kim (2016)

Machine learning Fractional Chern Insulator

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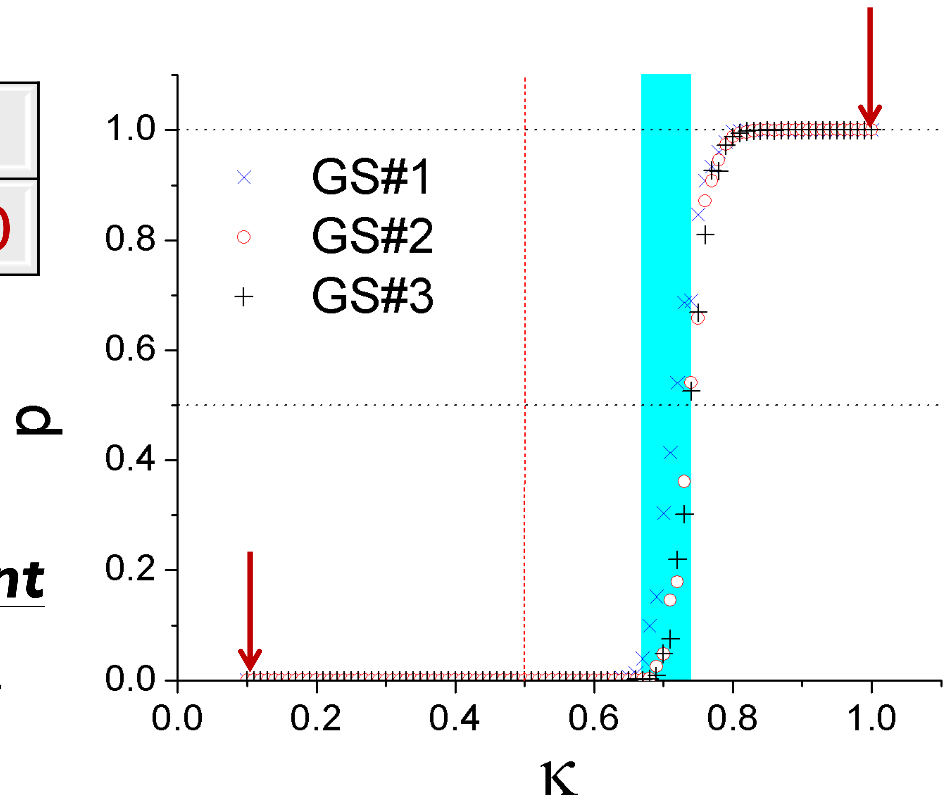


- κ_c~0.7 is ***consistent*** with our benchmark.

- captures ***all*** three ***degenerate ground states***

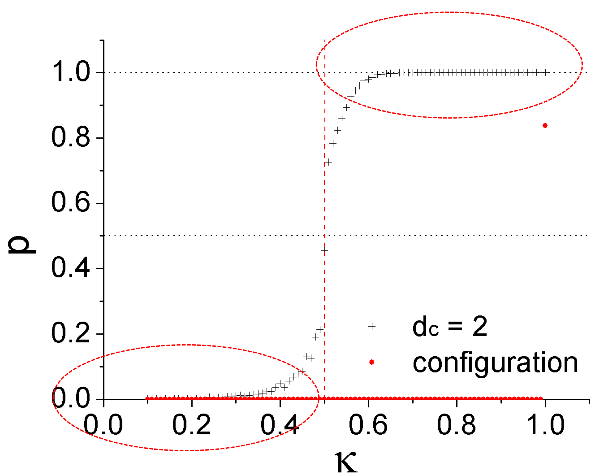
YZ, Eun-Ah Kim (2016)

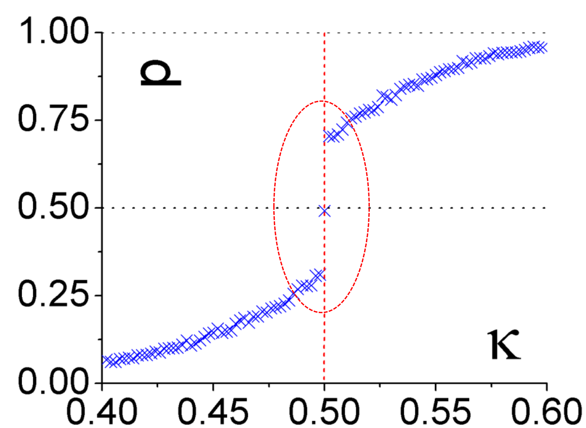
Why Quantum Loop Topography?

Advantages of Machine Learning

- Neural network can also distinguish ***different topological phases*** (e.g. FCI vs CI) as well as ***different topological indices*** (e.g. ν=1 vs ν=-1 and ν=2).

- ***Accuracy*** on both phases and transitions





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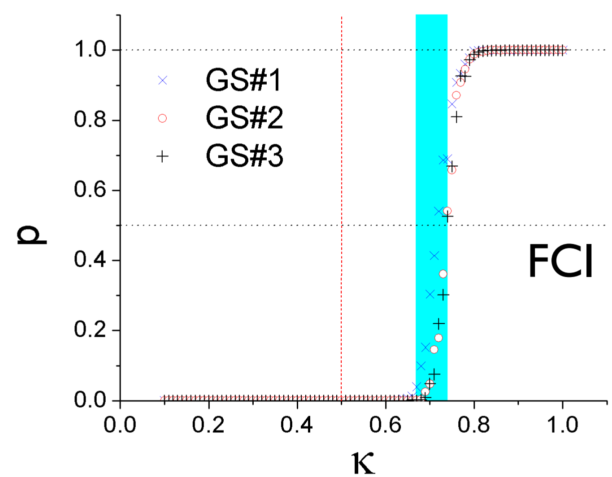

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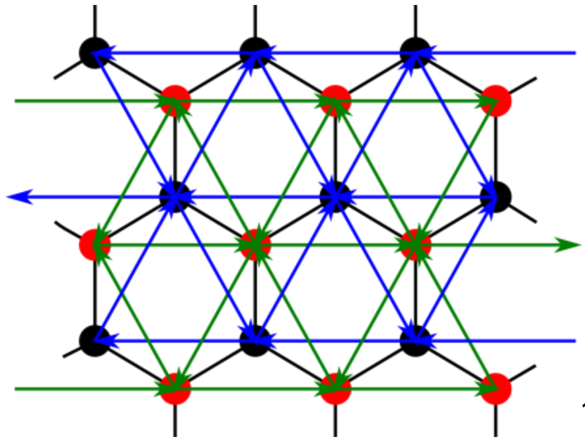
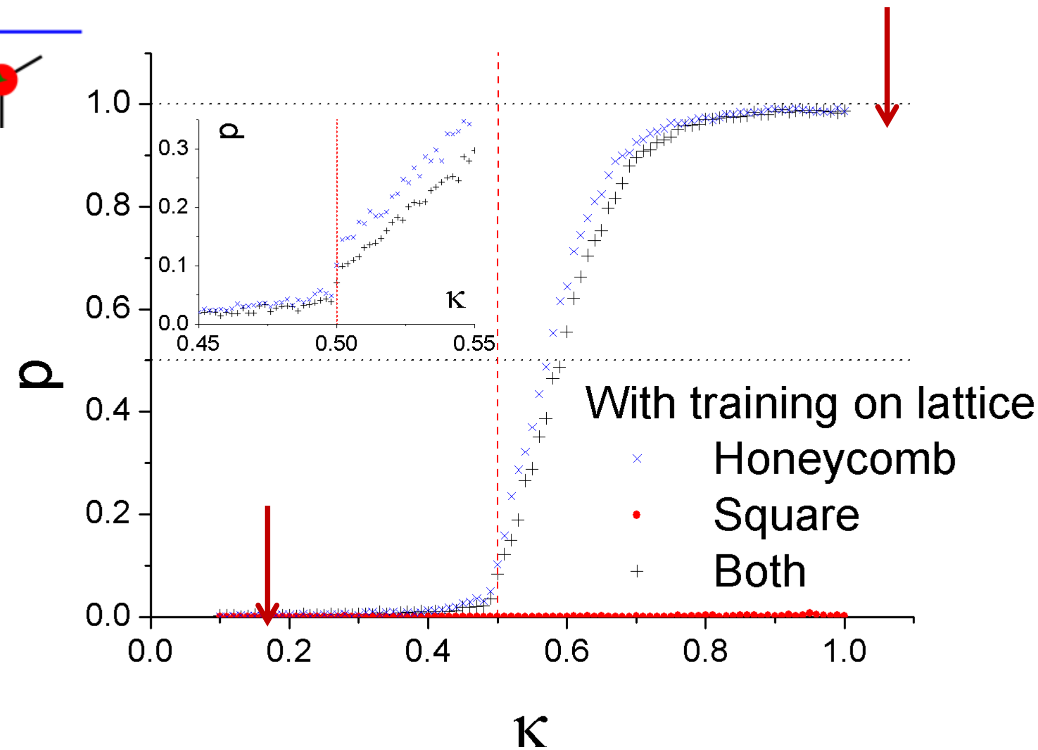
- ***Accuracy*** on both phases and transitions

- ***Efficiency***, and no more Monte Carlo averaging

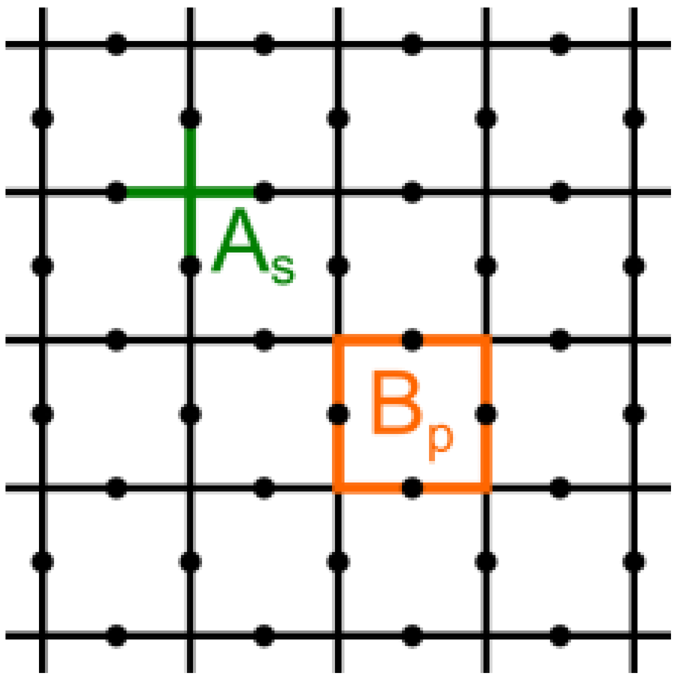
- ***Generalizability and Versatility***: one trained neural network for all degenerate ground states, all parameters in the phase diagram, lattice structures and symmetries, and more…

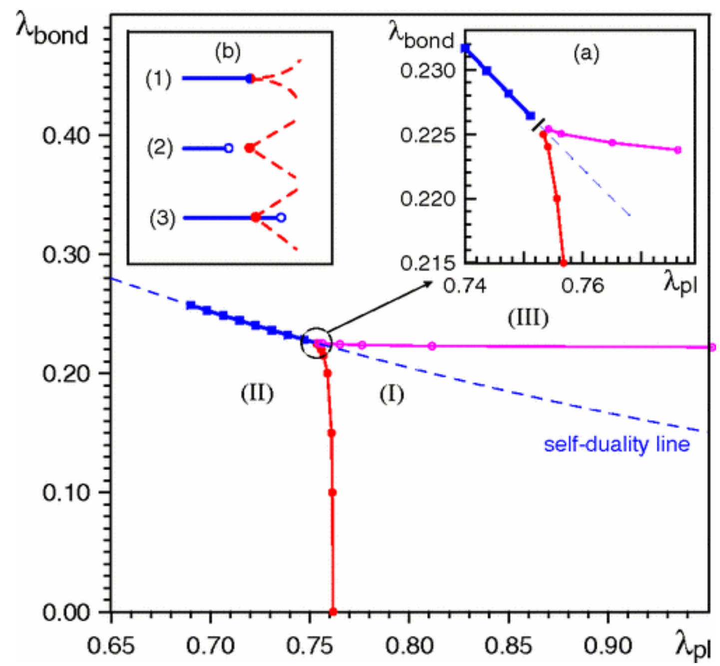
Cross training lattice symmetries





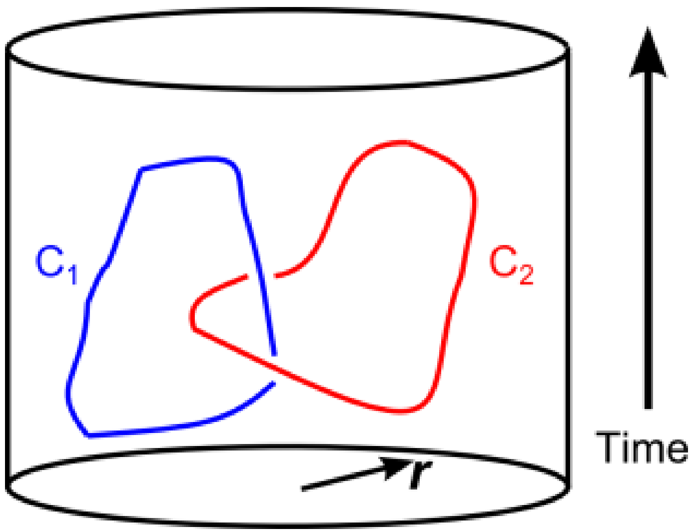
Machine learning Z_2 quantum spin liquid





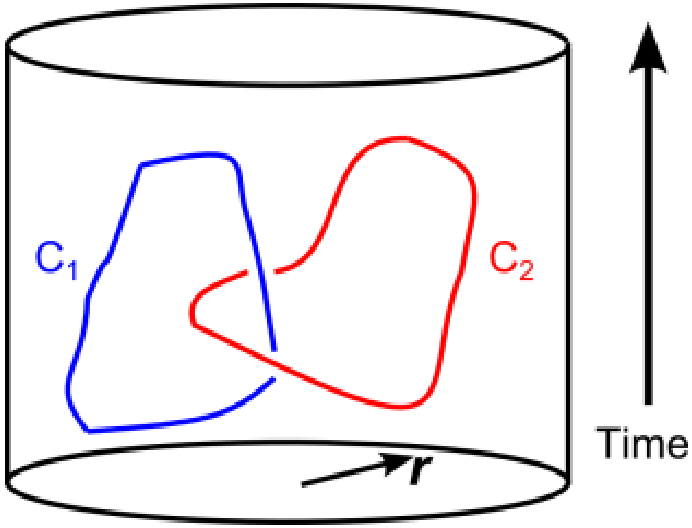
I. S. Tupitsyn, A. Kitaev, N.V. Prokof'ev, and P. C. E. Stamp (2010).

Machine learning Z_2 quantum spin liquid

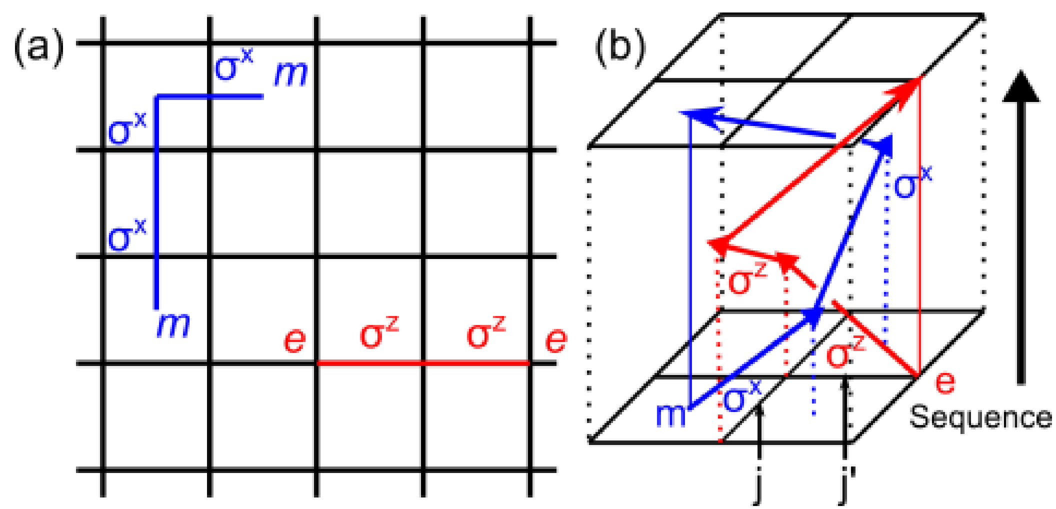


Dream theory

Machine learning Z_2 quantum spin liquid

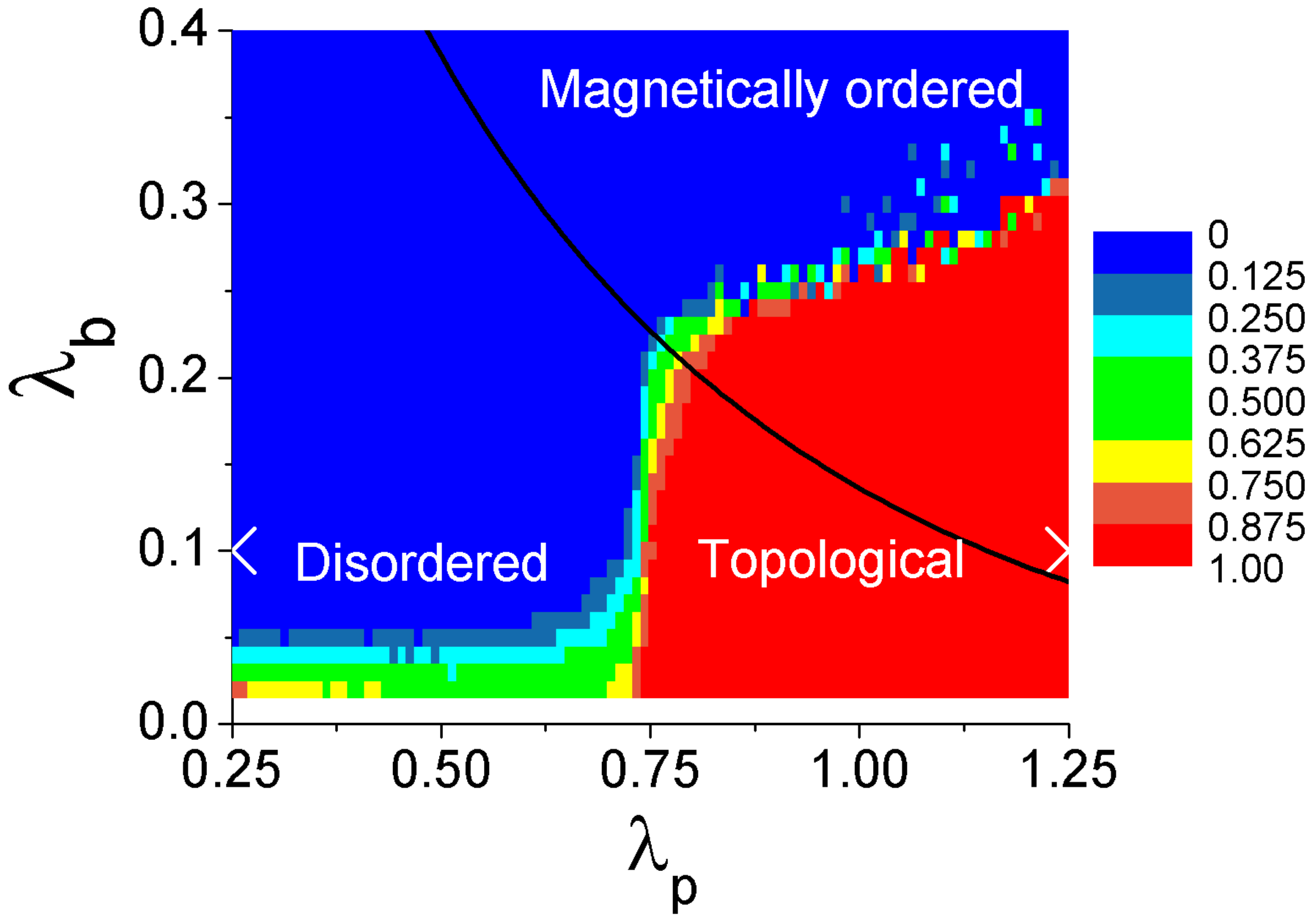


Dream theory



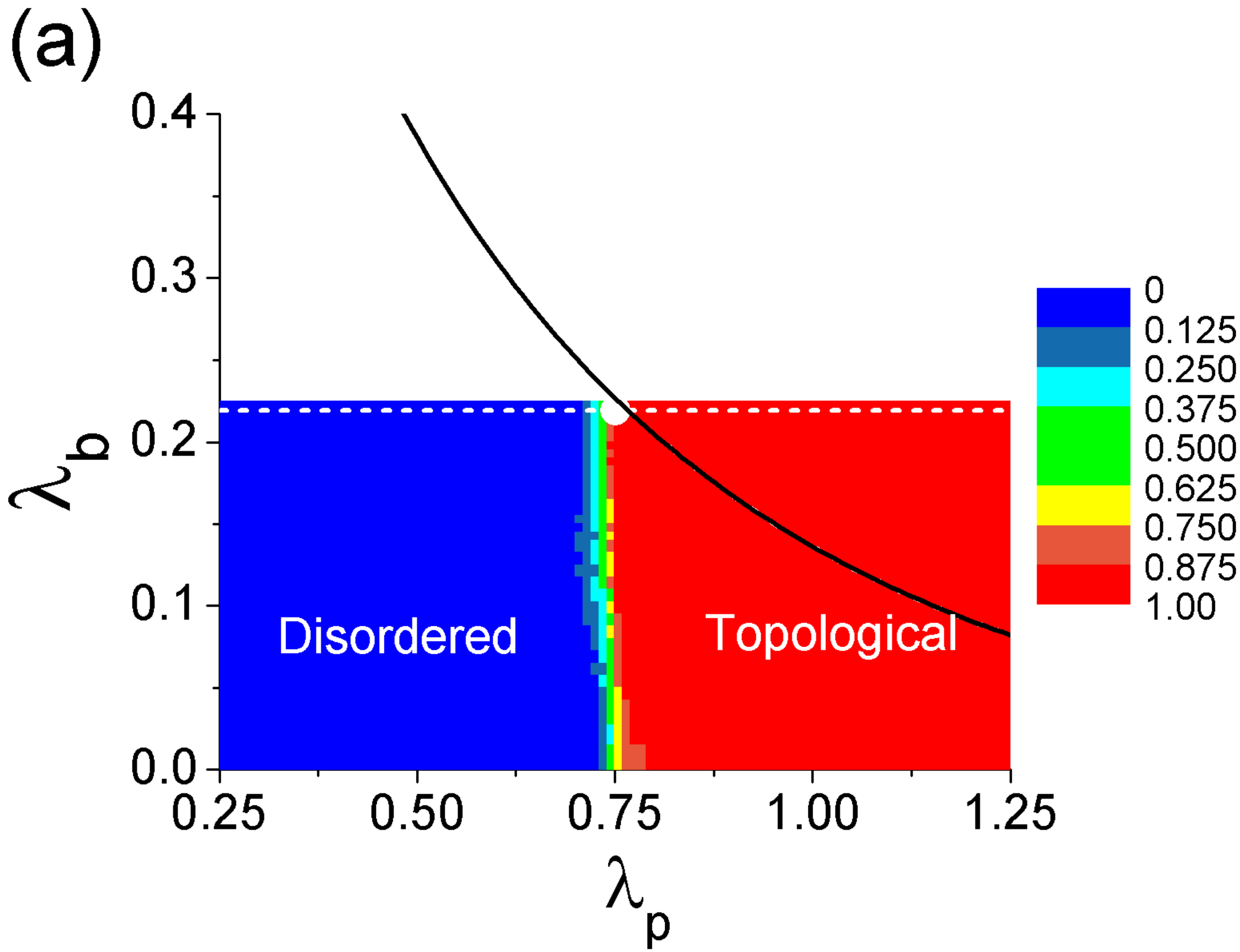
Reality

Machine learning Z_2 quantum spin liquid



YZ, R.G. Melko, Eun-Ah Kim (2017)

Machine learning Z_2 quantum spin liquid



YZ, R.G. Melko, Eun-Ah Kim (2017)

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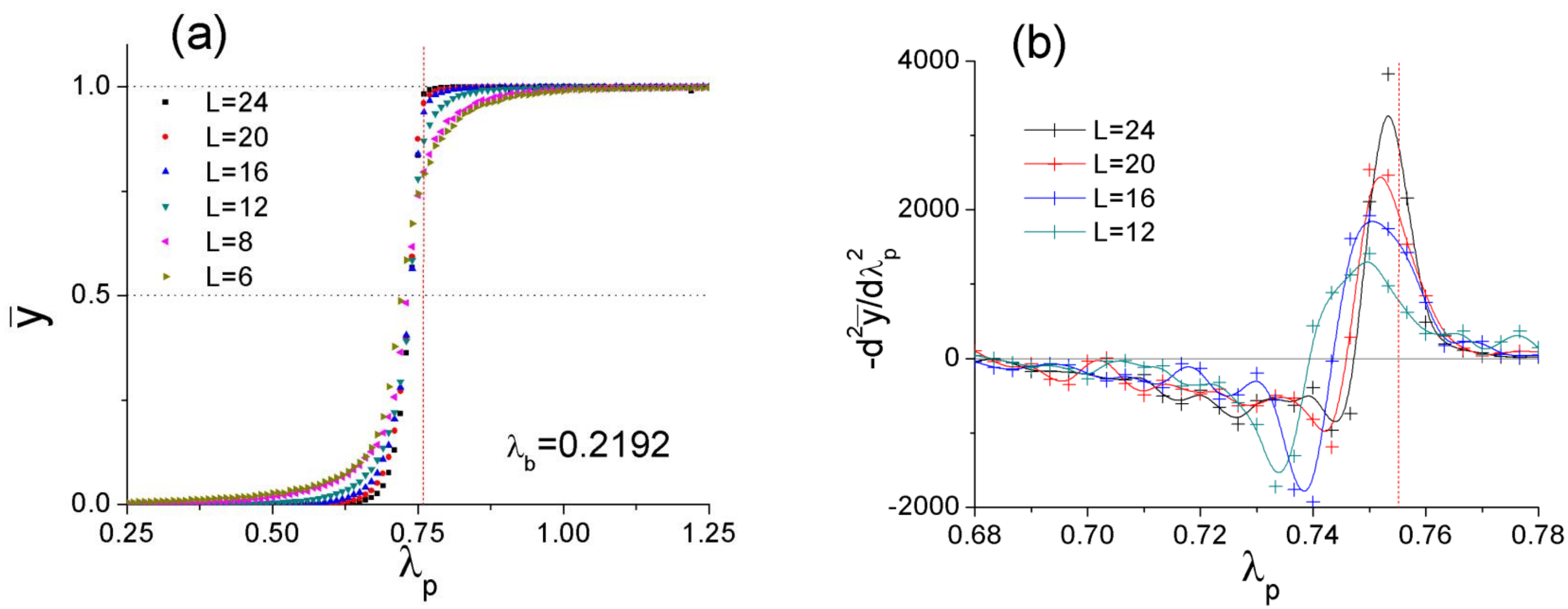
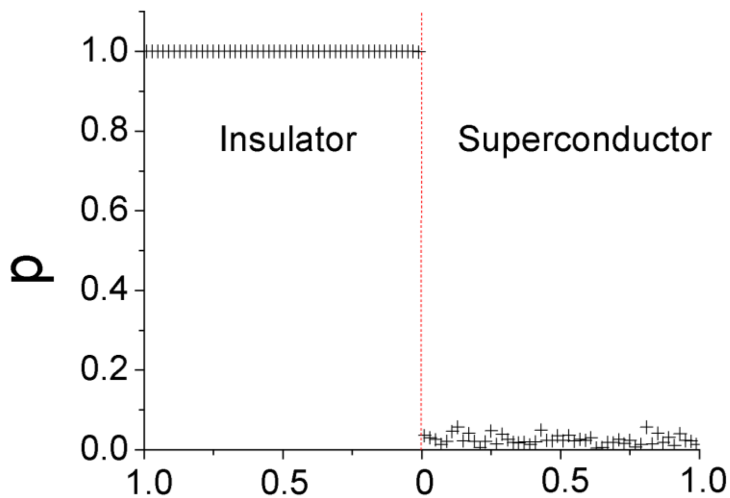


YZ, R.G. Melko, Eun-Ah Kim (2017)

And more …



- Meissner effect for ***superconductivity***

Unpublished data

Condensed Matter Physics in the present

Things we have

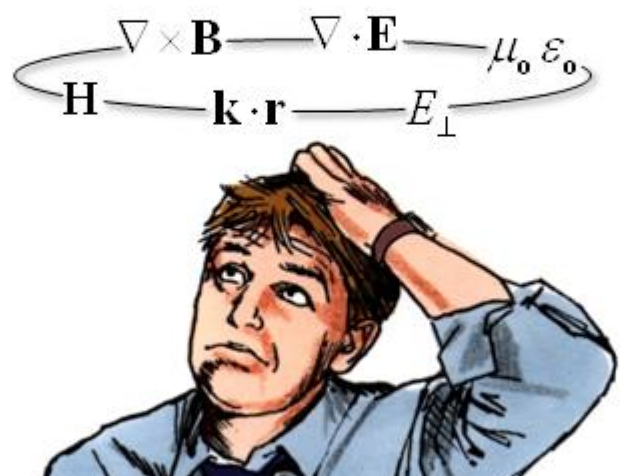
- Characteristics of the phase
- Known models (exp samples)

THE heavy lifting

- Approximations, renormalization group, numerical calculations, exp samples, materials, new tech & setup...

Things we want

- Phase diagram (Universality class)
- Phase transitions



Condensed Matter Physics in the ‘future’

Things we have

Characteristics of the phase

Known models (exp samples)

Machine learning DOES heavy lifting

Quantum Loop Topography

Neural network

Things we want

Phase diagram (Universality class)

Phase transitions

What's next?

- Generalizations and applications to topological phases and beyond
- Gapless systems and quantum criticality

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  - Entanglement
  - Scanning tunneling experiments and design, etc.

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- Generalizations and applications to topological phases and beyond
- Gapless systems and quantum criticality
- Alternative junctions in place of or additional models of quantum loop topography
  - Entanglement
  - Scanning tunneling experiments and design, etc.
- Reverse engineering machine learning – from neural network to condense matter theory

Summary

- Quantum Loop Topography as a bridge (feature selection layer) between the physical theories and machine learning technology

- Examples of machine learning topological phases, such as Chern insulator, fractional Chern insulator, and Z_2 quantum spin liquid

- Advantages of machine learning quantum phases with quantum loop topography:
    - Accuracy
    - Efficiency
    - Versatility

- The story is just beginning…