Learning Quantum Emergence

- Objectively quantify macroscopic property

e.g. Magnetization

Material

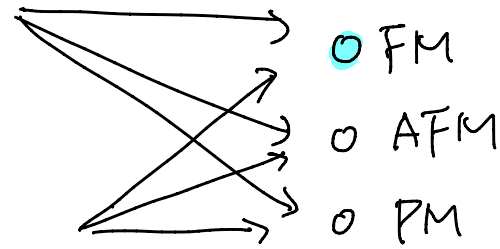
Magnetometry Data

$M(T, B, \vec{r})$

$\Updownarrow$

Model many body $\hat{H}$

& synthetic Data



$$\sum_i \langle \sigma_i \rangle = \frac{1}{Z} \mathrm{Tr} \sum_i \sigma_i e^{-\beta \hat{H}}$$

$$= \langle \Psi | \sum_i \sigma_i | \Psi \rangle$$

at $T=0$, for a unique G.S. $|\Psi\rangle$

- Learning: Compress Knowledge to Abstract Emergence (Diagnose)

$$G_{xy} = \frac{dI_x}{dV_y}(T, \vec{B}, P, \cdots)$$

LDOS $\propto \frac{dI_{tun.}}{dV}(\vec{r}, T, \vec{B}, P, \cdots)$ $\xrightarrow{\text{Regression}}$ Symmetry breaking

Scattering intensity $S(\vec{q}, \omega, T, \cdots)$ $\xleftarrow{\text{Generative Modeling}}$ Topological order

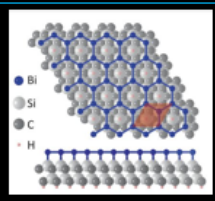
Density Matrix — Many body localization

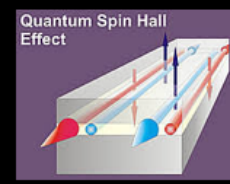
Many-body wave function

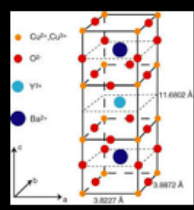
$\boxed{\text{Complex Data}}$ $\boxed{\text{Compact, abstract principles}}$

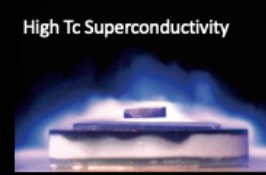
✱ Data Driven Challenges

Quantum Emergence: New State of Many Electrons









Over trillion trillion individual electrons

Learning Quantum Emergence

Complex Reality of Data

Simple Principles

$dI/dV(\vec{r}, V, T, \delta)$

$S(\vec{q}, T, p, \vec{B}, \ldots)$

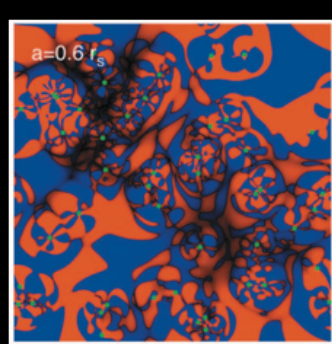
Many-body WF

$i\hbar \frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle$

Quantum Complexity

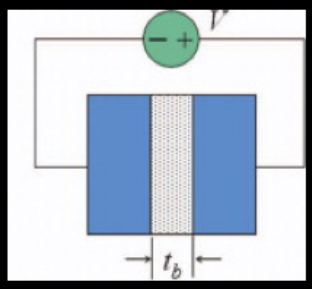
Symmetry Breaking
Topological Invariant

Complexity of Quantum Many-body State

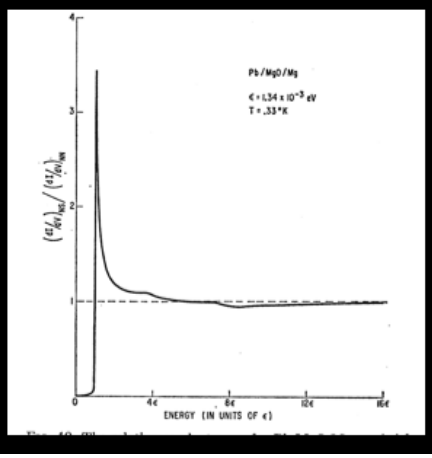


Many body wave function of 49 electrons:
a function in trillion trillion trillion trillion dimensional space

Tunneling Density of States, in 1962



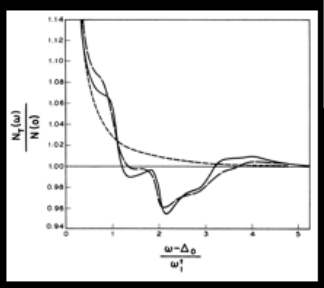
Differential conductance dI/dV @ V proportional to N(E=eV)



Giaever et al, Phys. Rev. 126, 941 (1962)

Generative Model

Schrieffer, Scalapino, Wilkins, PRL 10, 336 (1963)

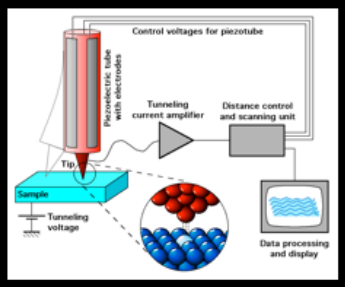


EFFECTIVE TUNNELING DENSITY OF STATES IN SUPERCONDUCTORS*

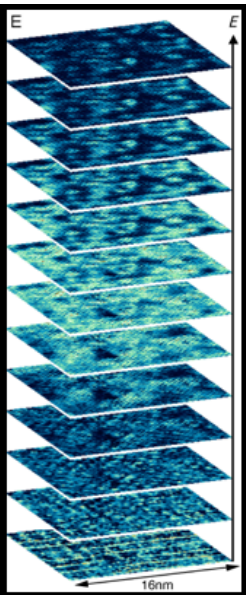
J. R. Schrieffer, D. J. Scalapino, and J. W. Wilkins
University of Pennsylvania, Philadelphia, Pennsylvania
(Received 15 March 1963)

$$\frac{dI_s(V)}{dV}\Big/\frac{dI_n(V)}{dV} = \frac{N_\Gamma(V)}{N(0)} = \mathrm{Re}\left\{\frac{V}{[V^2-\Delta^2(V)]^{1/2}}\right\}.$$

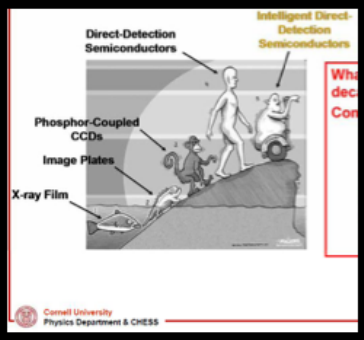
Tunneling Density of States, in 2000's



Imaging N(r,E): Scanning Tunneling Spectroscopy



Comprehensive Data with Modern Detectors

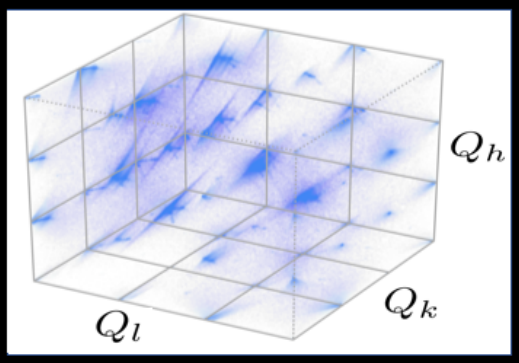


High energy X-ray Data at CHESS
> Possibly 5 TB per day

https://neutrons.ornl.gov/sequoia

Neutron data from Spallation Neutron Source
> Possibly 200 GB per hour

Data-driven challenges in Reciprocal Space



Diffuse Scattering data on 1T-TiSe2 at 150 K (CDW Tc~190K), courtesy Jacob Ruff (CHESS)

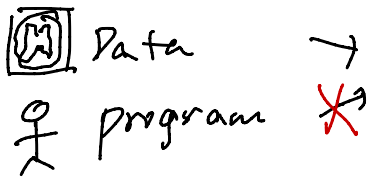
(T, p, δ)

(T, p, δ)

☐ Machine Learning Approach to Data Science

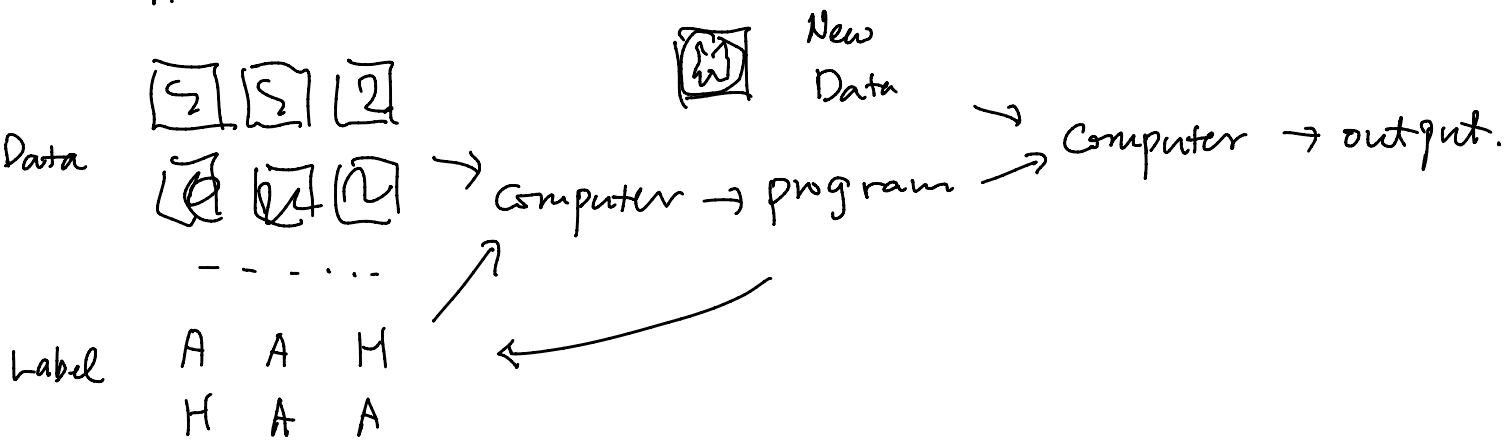
- problem: Diagnose Altzheimer from an MRI scan
  " Quantum Spin Liquid " Quantum Matter
  Loop order Data.

- Manual approach



→ Computer → output.

- ML approach: learn from ∃ "labeled data"

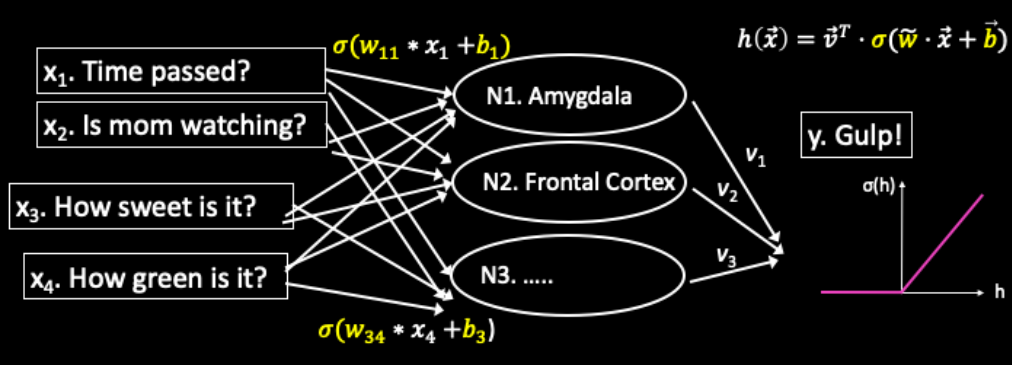


☆ Supervised ML (w/ a shallow ANN)

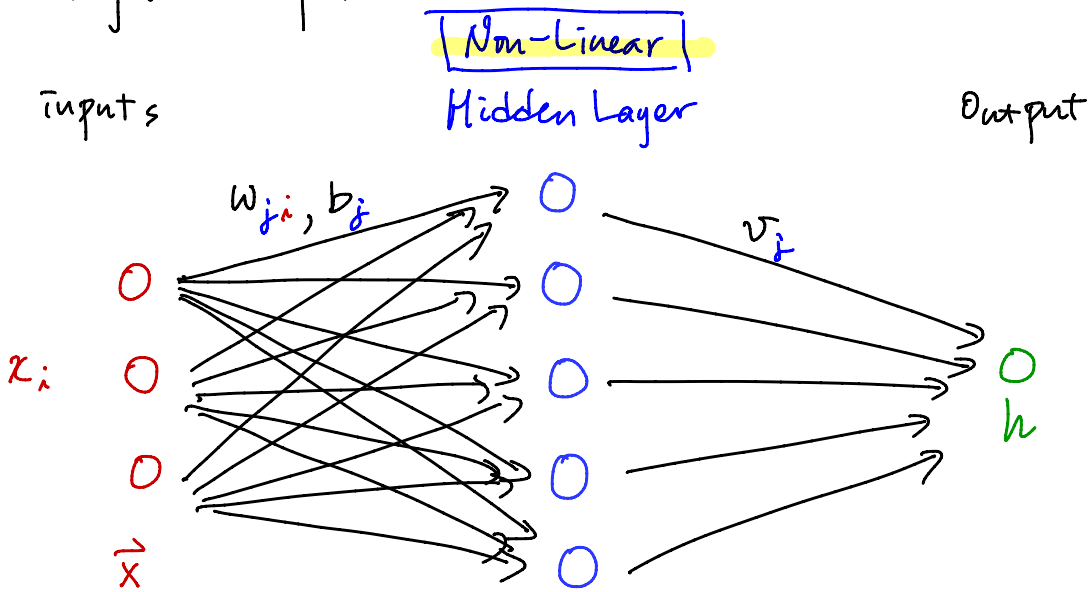
Supervised ML

Kids' decision upon dropping food....

Determined by w(t) and b(t)

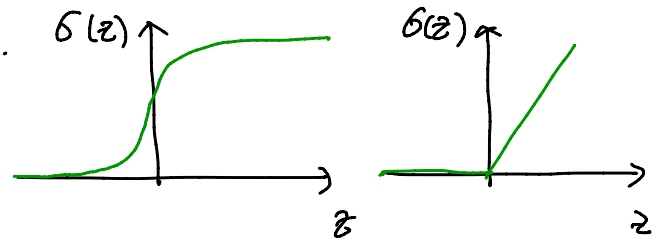


□ Multi-layer Perceptron



$$h(\vec{x}) = \sigma\left(\vec{v}^T \cdot \sigma(\tilde{w} \cdot \vec{x} + \vec{b})\right)$$

$\sigma(z)$: non-linear activation function.



① Hidden layer is necessary for non-linearity

⇒ First multi-layer perceptron by F. Rosenblatt at Cornell.

✱ - Demo : Power of non-linearity, expressive.

https://github.com/iamc/ML-CM-2019/blob/master/Eun-Ah_Kim/Example_linearvsRELUclassifier.ipynb

See that ① linear classification fails with perceptron

③ A single hidden Layer leads to success

② Does not generalize outside of the range of data.

② Theorem: Universal Approximation Theorem.

G. Cybenko (1989) Mathematics of Control, Signals, & Systems, 2(4), 303-314

☆ Demo: Interactive. Change Hidden Layer neuron #.

https://github.com/iamc/ML-CM-2019/blob/master/Eun-Ah_Kim/1-n-1.interactive.ipynb

- Check the increased expressibility upon increasing # of hidden layer neurons.

  Try suggesting data points with some non-linear function in mind.

  i) Set # of hidden layer neurons at 5 : put the # in the box and hit enter.

  ii) update the above to larger #'s

- Experience overfitting:

  Try suggesting data points with a linear distribution in mind.

  Set the # of hidden layer neurons at 30 and notice overfitting.

✱ Quantum Matter Data v.s. Classic (Classical) Data.

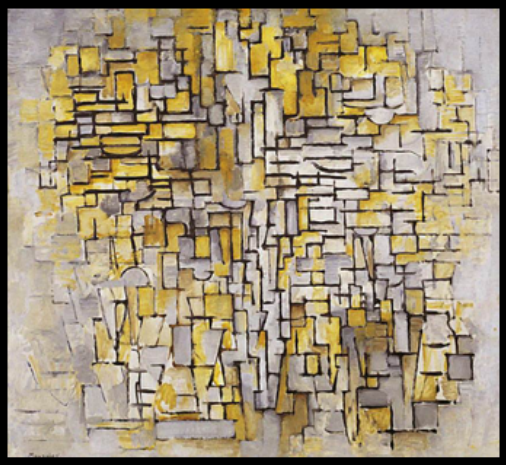
A Classic Image

Boticelli,
The Birth of Venus
(c. 1484-86)

- Local connectivity
- Clearly shaped boundary

➢ Keys for ConvNet's success

A Modern Art

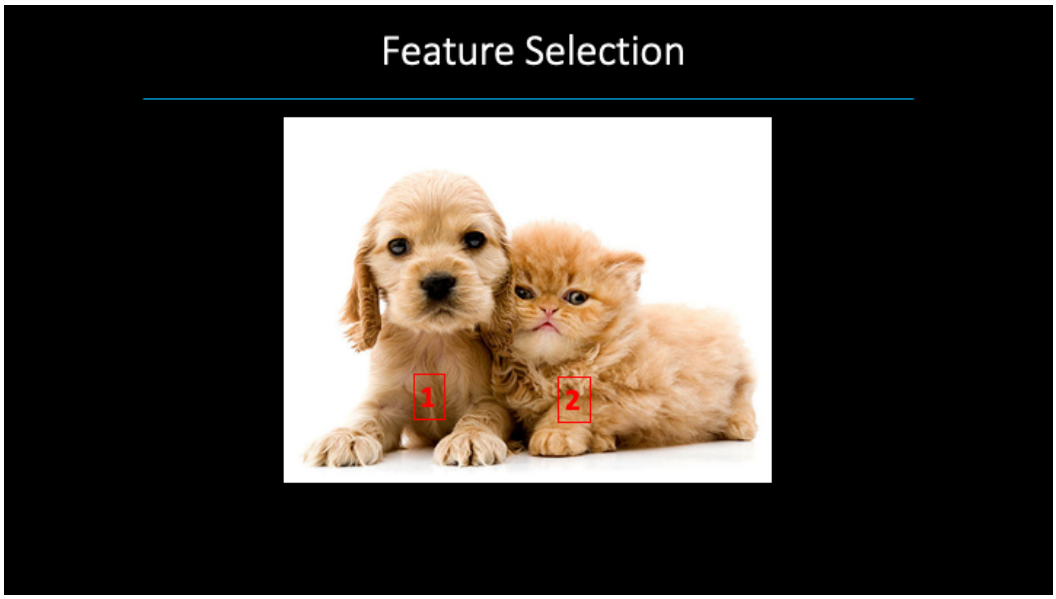


Mondrian,
Composition No. VII
(1913)

A Modern Art

Mondrian,
The Gray Tree (1912)

☆ Importance of physcis (domain-knowledge) guided feature selection



⇒ Quantum Loop Topography
: physics insight driven feature selection

✱ Supervised ML on Synthetic Data

Learn Chern number and Wilson Loops

Yi Zhang (Beking U)

Mike Matty (Cornell)

R. Melko (Waterloo)

Zlatko Papic (U of Leed)

Paul Ginsparg (Cornell)

Featured in Physics | Editors' Suggestion

Quantum Loop Topography for Machine Learning

Yi Zhang and Eun-Ah Kim
Phys. Rev. Lett. **118**, 216401 – Published 22 May 2017

Physics See Viewpoint: Neural Networks Identify Topological Phases

Machine Learning Z2 Quantum Spin Liquids with Quasi-particle Statistics, PRB 96, 245119 (2017)

Multi-faceted machine learning of competing orders in disordered interacting systems, arXiv: 1901.04079

Interpreting ML of Topological Phases, Zhang et al, In prep.

Learn Transport from Imaginary Time Data

G. Trey Driskell (Cornell)

S. Lederer (Cornell)

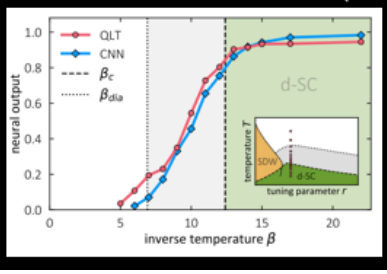
Yi Zhang (Peking U)

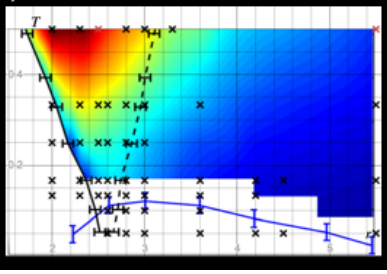
C. Bauer (Cologne)

S. Trebst (Cologne)

Zhang et al, PRB 99, 161120 (R)

Driskell et al, in prep.





Recognize Transition between Out of Equilibrium States

Jordan Venderley

Vedika Khemani (Harvard)

MENU nature materials

News & Views | Published: 24 July 2018

MATERIALS WITNESS

Learning from scratch

Philip Ball

Nature Materials **17**, 660 (2018) | Download Citation

PHYSICAL REVIEW LETTERS **120,** 257204 (2018)

Machine Learning Out-of-Equilibrium Phases of Matter

Jordan Venderley,[1] Vedika Khemani,[2] and Eun-Ah Kim[1]
[1]*Department of Physics, Cornell University, Ithaca, New York 14853, USA*
[2]*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*

□ Quantum Loop Topography for Chern Insulator

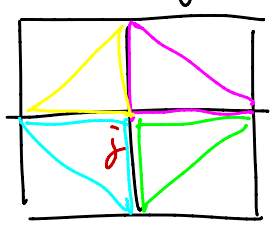
- Quantum Loop Topography

  : Feature Selection Guided by Physical Insight (Domain Knowledge)

  on quantum MC instances of wave function (VMC) or thermal ensemble (QMC)

  Given site j,

  Consider $\forall$ triangles $\triangle_{jkl}$ of given lateral dimension.



  $\Rightarrow$ For each triangle $\triangle_{jkl}$, enter $\tilde{P}_{jk}|_\alpha \, \tilde{P}_{kl}|_\beta \, \tilde{P}_{lj}|_\gamma$ into the input vector $\vec{x}$ where $\tilde{P}_{kl}|_\beta \equiv \langle c_k^\dagger c_l \rangle_\beta$ for a MC instance β.

  ① MC Greens function's are selected & organized

  ② # of complex valued entries per site : $D(d_c)$ depends on lattice & cut off d_c.
  e.g. square lattice w/ $d_c = 1$, $D(d_c) = 4$.
  $\Rightarrow$ quasi-2D "image"

  ③ Position space-based $\rightarrow$ handle disorder.

- QLT vs σ_{xy}: physical insight (Domain Knowledge)

① Kubo formula for σ_{xy} at $T=0$

$$\sigma_{xy} = \frac{ie^2\hbar}{N} \sum_{n\neq 0} \left[\frac{\langle \Phi_0 | v_y | \Phi_n \rangle \langle \Phi_n | v_x | \Phi_0 \rangle - (x \leftrightarrow y)}{(E_n - E_0)^2} \right]$$

For free fermions, $|\Phi_0\rangle = \prod_{m\in v} |m\rangle$, $|m\rangle$: single ptl state.

$\leftarrow$ valence band.

$$\sigma_{xy} = \frac{ie^2\hbar}{N} \sum_{m\in v} \sum_{n\notin v} \left[\frac{\langle m | v_y | n \rangle \langle n | v_x | m \rangle - (x \leftrightarrow y)}{(\varepsilon_n - \varepsilon_m)^2} \right]$$

② Consider $\hat{P} = \sum_{m\in v} |m\rangle\langle m|$ and a flat band Hamiltonian

$\hat{H}' = -\Delta \hat{P}$ with a gap Δ.

$\Rightarrow$ $\hat{H}'$ is adiabatically connected to the system $\hat{H}$ if $\hat{H}$ is gapped.

③
$$\begin{aligned}
\langle c_i^\dagger c_j \rangle &= \prod_{m\in v} \langle m | c_i^\dagger c_j \prod_{m'} | m \rangle \\
&= \sum_m \langle m | c_i^\dagger c_j | m \rangle \\
&= \sum_{r,r'} \sum_m \langle m | r \rangle \langle r | c_i^\dagger c_j | r' \rangle \langle r' | m \rangle \\
&= \sum_{r,r'} \sum_m \langle r' | m \rangle \langle m | r \rangle \langle 0 | c_r c_i^\dagger c_j c_{r'}^\dagger | 0 \rangle \\
&= \sum_{r,r'} \hat{P}_{rr'} \, \delta_{j,r'} \, \delta_{i,r} = \hat{P}_{ij}
\end{aligned}$$

④ $\tilde{v}_x(\vec{r}) = \frac{d\tilde{x}}{dt}(\vec{r}) \approx \frac{i}{\hbar}[H(\vec{r}), \hat{x}]$

$$= -\Delta \frac{i}{\hbar}[\hat{P}(\vec{r}), \hat{x}]$$

$$= -\Delta \frac{i}{\hbar}\sum_{r'} P_{r'r} c^{\dagger}_{r'} c_r (x - x')$$

⑤ $\sigma_{xy} = \frac{ie^2\hbar}{N\Delta} \mathrm{tr}\left[\hat{P} v_y (1-\hat{P}) v_x - \hat{P} v_x (1-\hat{P}) v_y\right]$

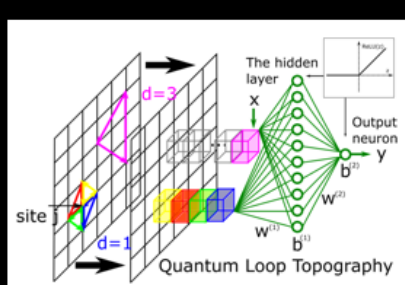
$$= \frac{-ie^2}{N\hbar} \mathrm{tr}\left[\hat{P}[\hat{P}, y][\hat{P}, x] - \hat{P}[\hat{P}, x][\hat{P}, y]\right]$$

$$= \frac{e^2}{\hbar}\frac{1}{N} i P_{jk} P_{kl} P_{lj}\left[(\vec{r}_k - \vec{r}_l) \times (\vec{r}_j - \vec{r}_l) \cdot \hat{z}\right]$$

$$= \frac{e^2}{h}\frac{1}{N} 4\pi i P_{jk} P_{kl} P_{lj} S \Delta_{jkl}$$

$\therefore$ $\tilde{P}_{jk}|_\alpha \tilde{P}_{kl}|_\beta \tilde{P}_{lj}|_\gamma$: "snapshot" of fluctuating $P_{jk} P_{kl} P_{lj}$

Interpret ML of Chern Insulator



- QLT data entry for input **x**

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

for a particular MC config.

- Trained Network Expresses:

$$y = \sigma\left[\sum_j w_j^{(2)} \sigma\left(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)}\right) + b^{(2)}\right]$$