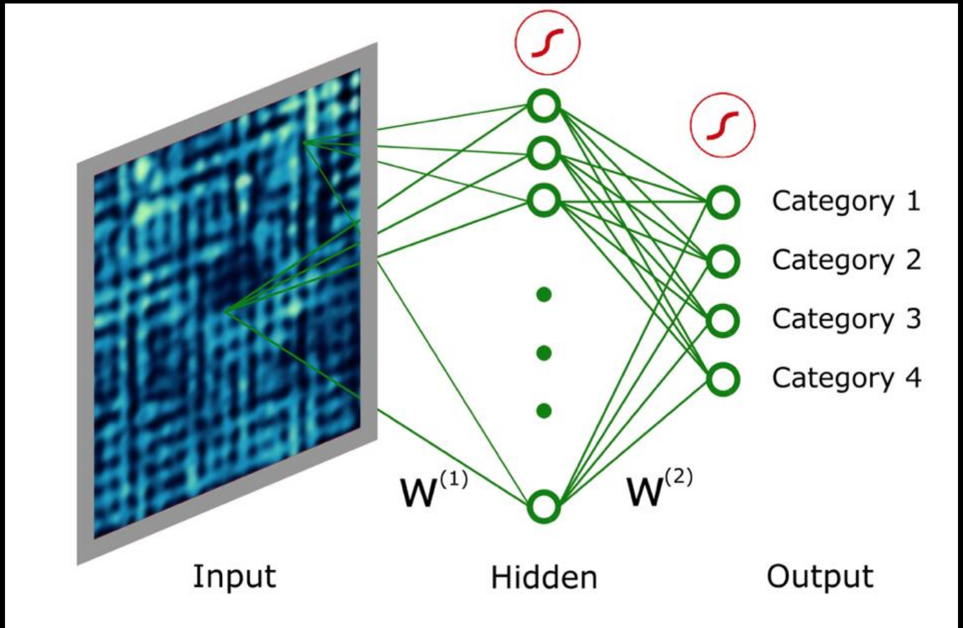
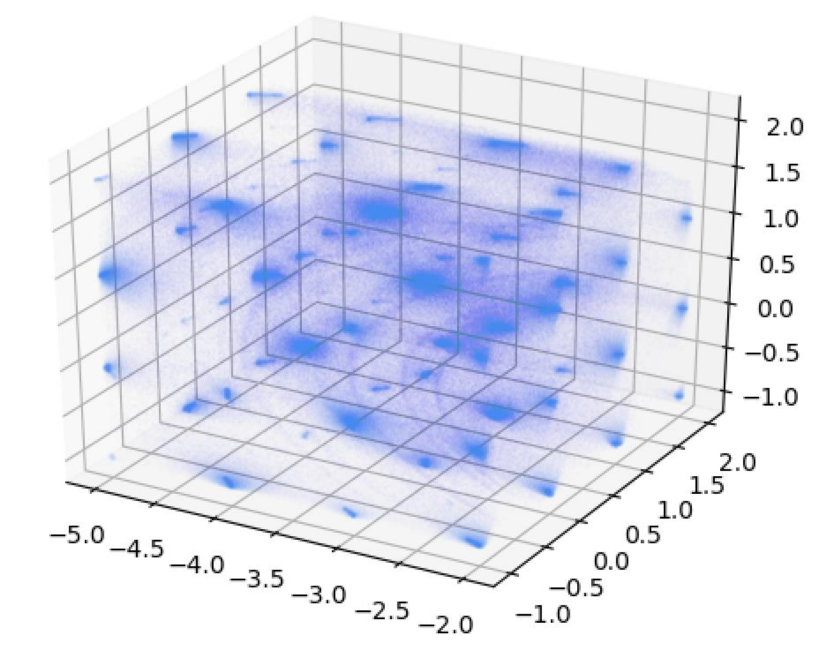
MachineLearning Quantum Emergence





Eun-Ah Kim (Cornell)

KITP, Feb14, 2019

CCMR

U.S. DEPARTMENT OF ENERGY

Learning Quantum Emergence

Complex Reality of Data

Simple Principles

Phase Diagrams
Many-body WF

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

Quantum Complexity

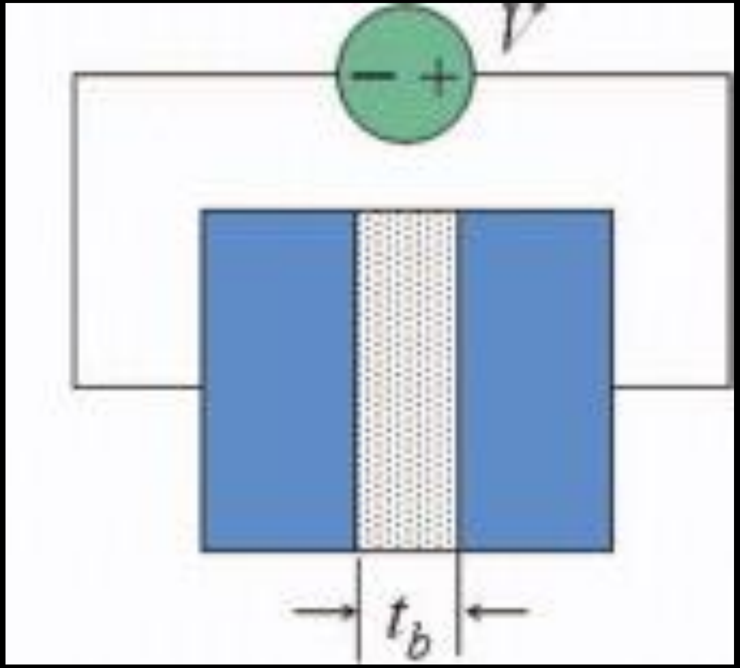
Entropy
Phonons
Topological Invariant
Fermi statistics

Data Driven Challenges

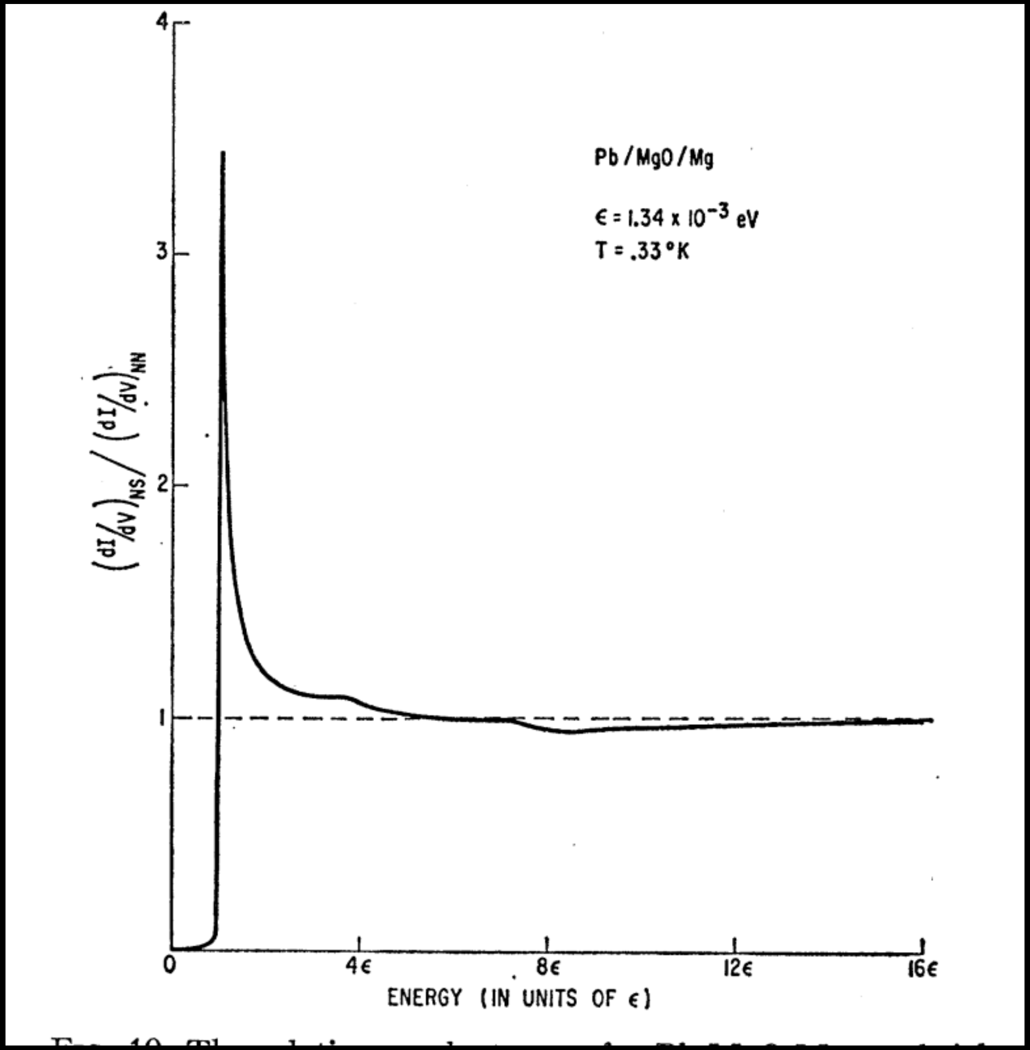
Complexity of Quantum Many-body State

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

Tunneling Density of States, in 1962



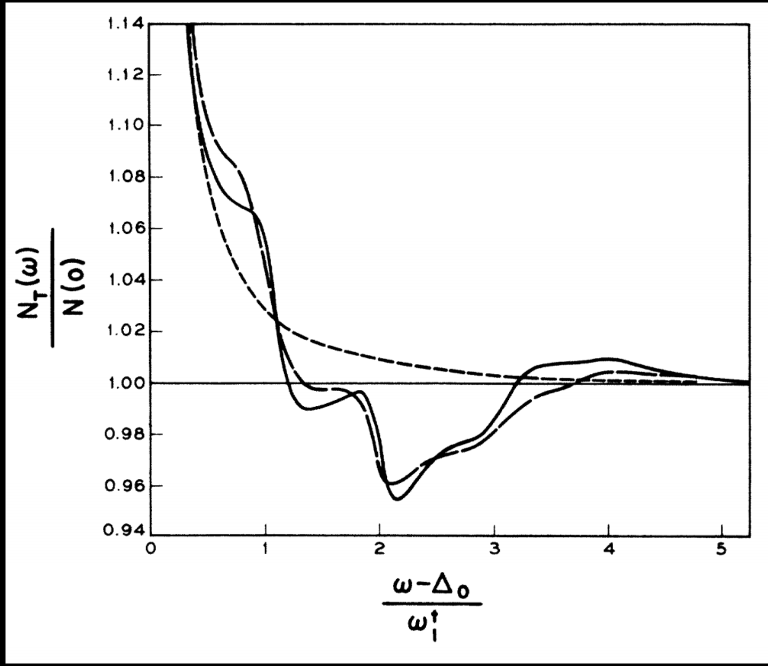
Differential conductance dI/dV @ V proportional to N(E=eV)



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

Generative Model

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

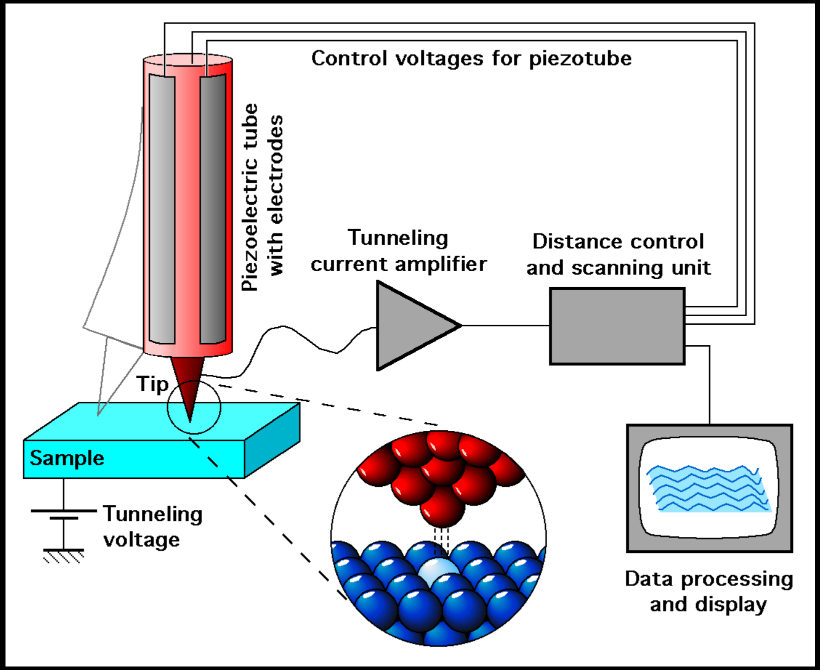


EFFECTIVE TUNNELING DENSITY OF STATES IN SUPERCONDUCTORS*

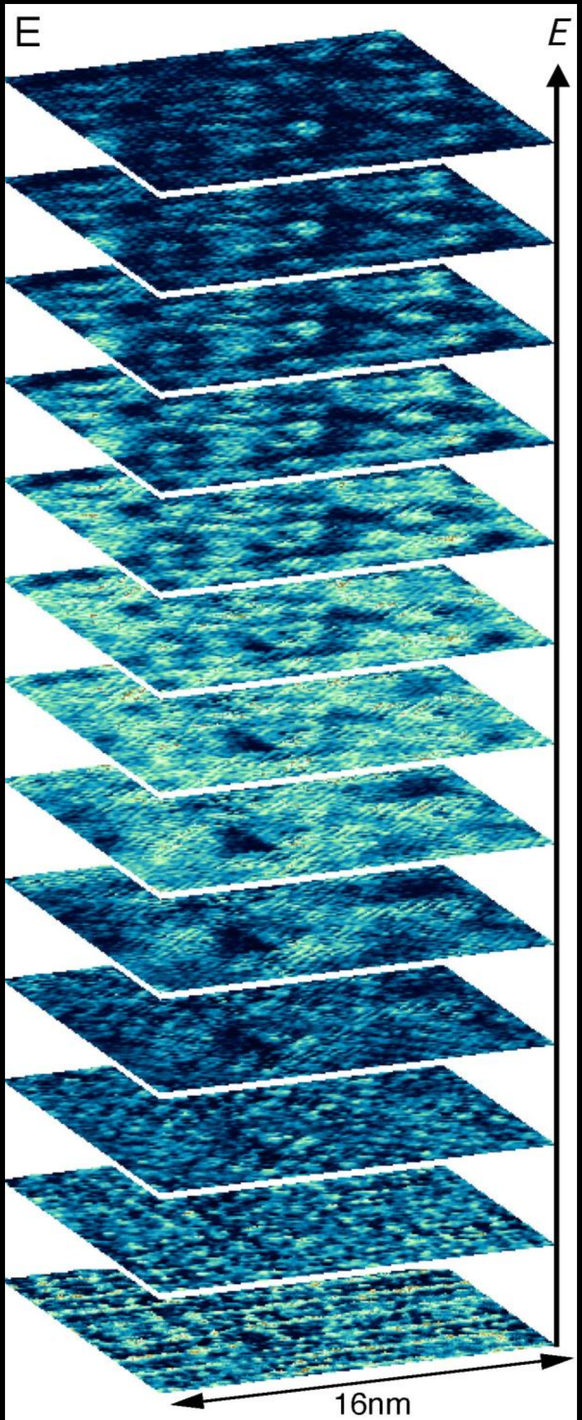
J. R. Schrieffer, D. J. Scalapino, and J. W. Wilkins
University of Pennsylvania, Philadelphia, Pennsylvania
(Received 15 March 1963)

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

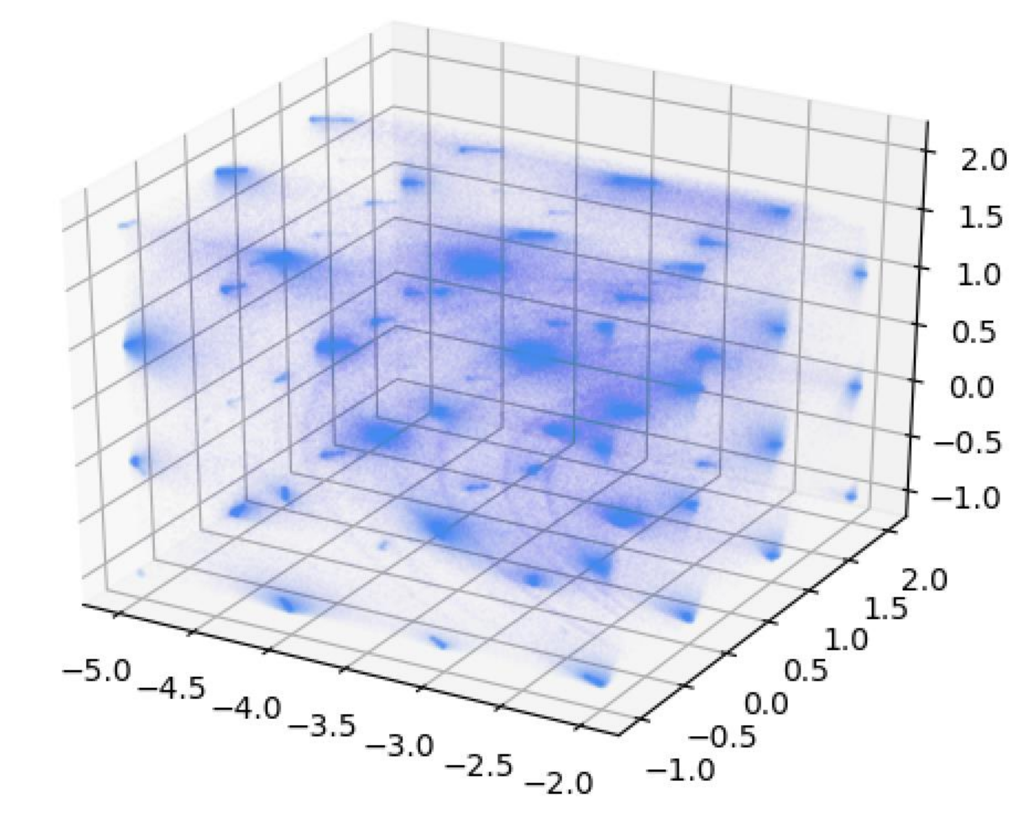
Tunneling Density of States, in 2000's



Imaging N(r,E):
Scanning Tunneling Spectroscopy

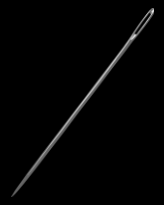


Data-driven challenges in Reciprocal Space



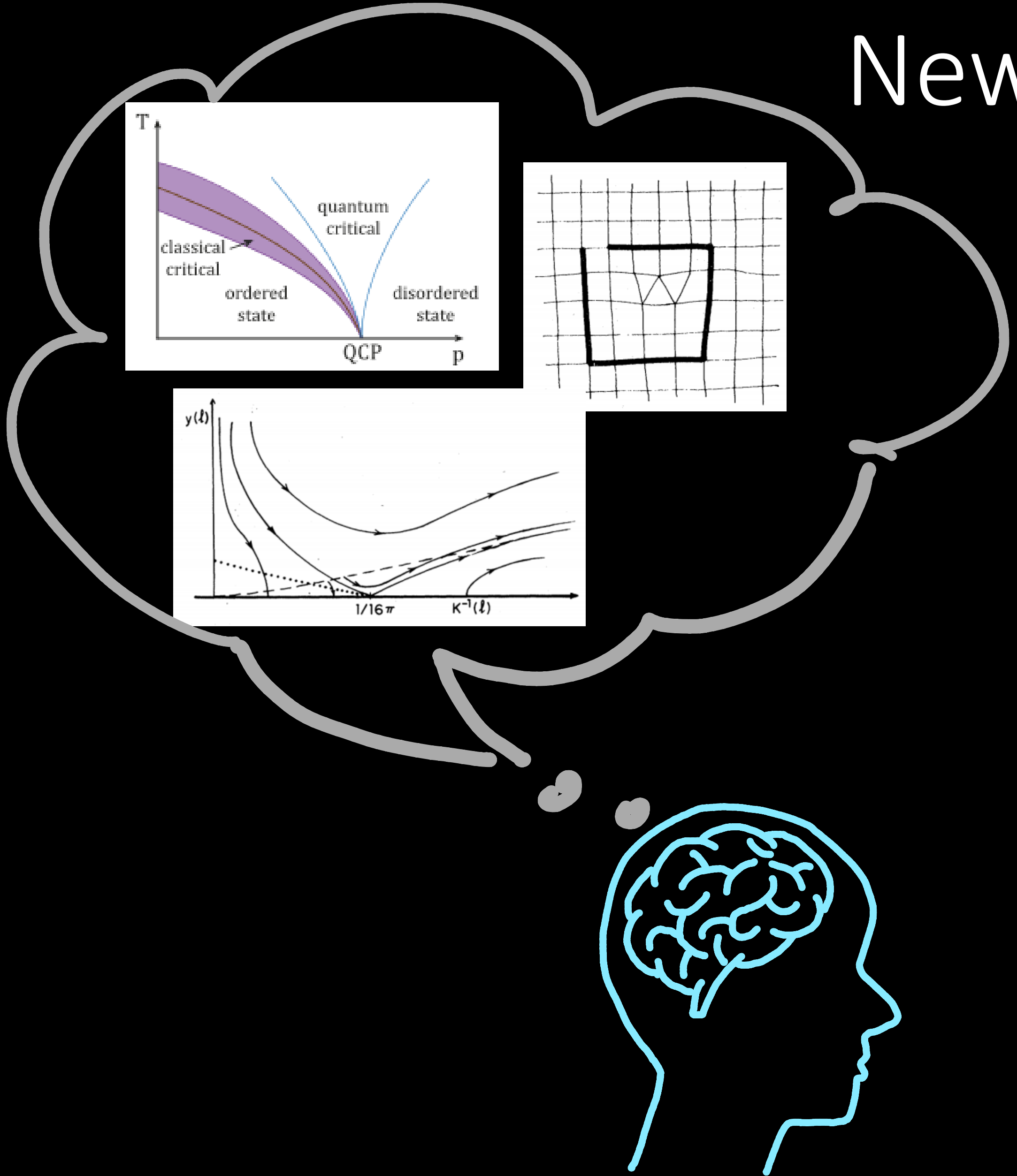
Diffuse Scattering data on $TiSe_2$ at 150 K (CDW Tc~190K), courtesy Jacob Ruff (CHESS)

(T, p, δ)

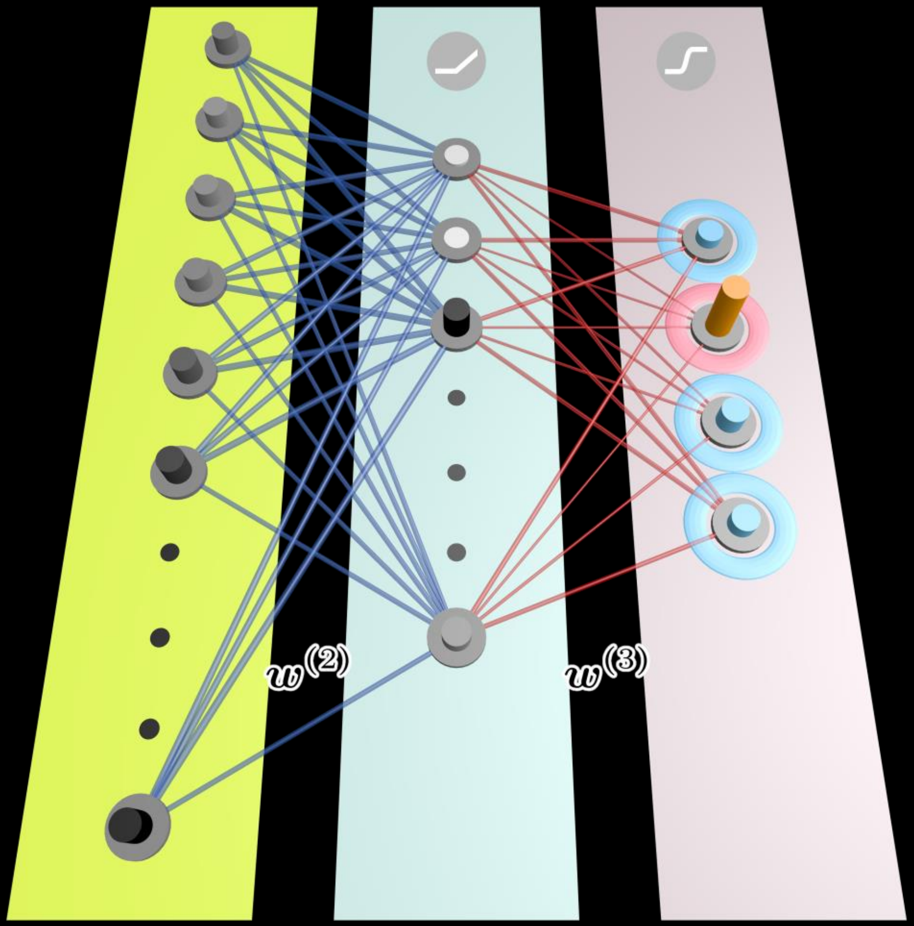


(T, p, δ)

New Insight through Synergy

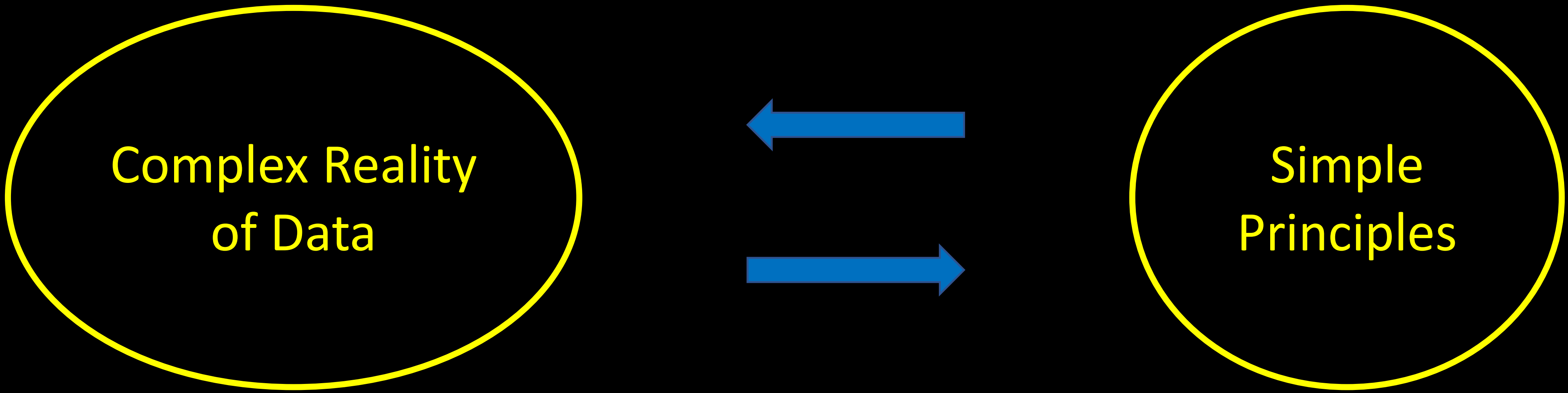


⊗

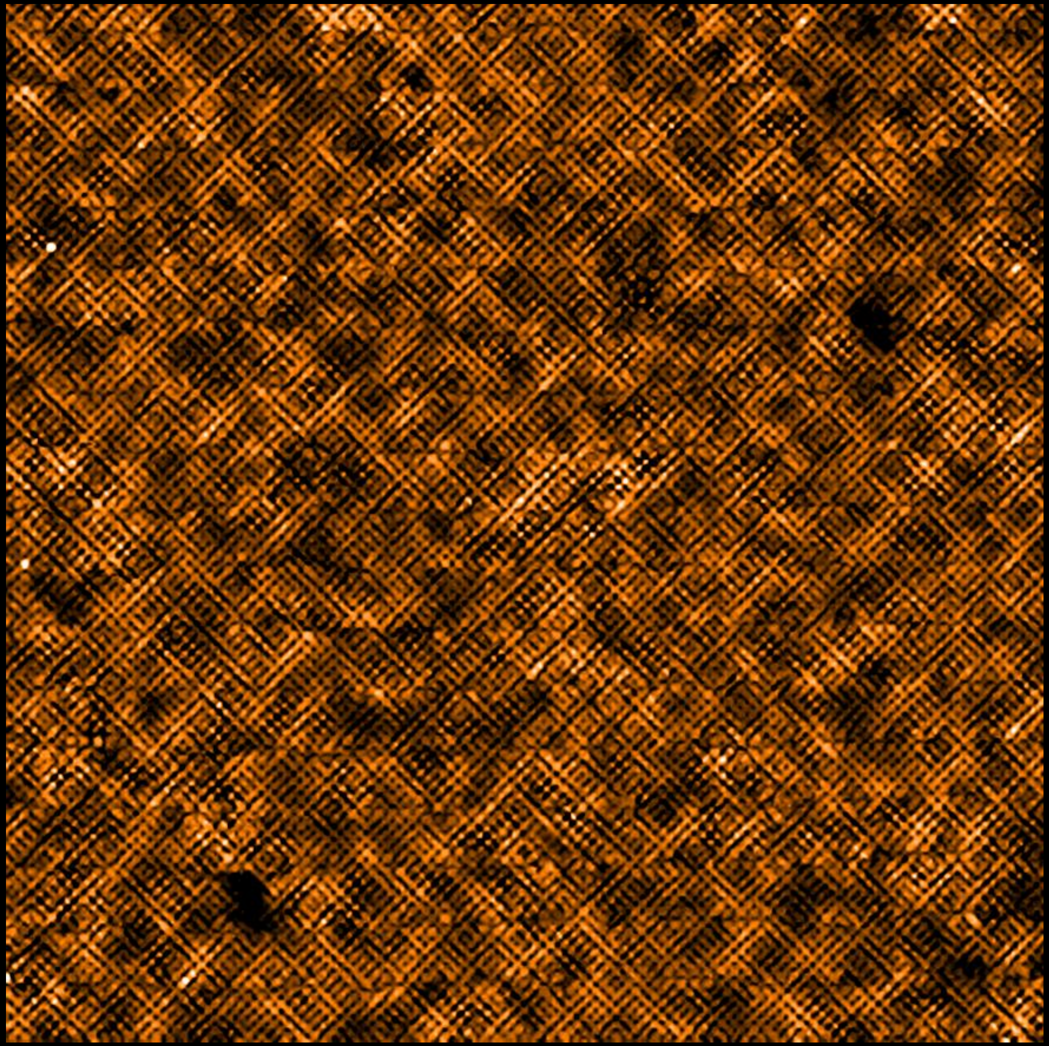


Supervised ML for Hypothesis Test

Learning Quantum Emergence



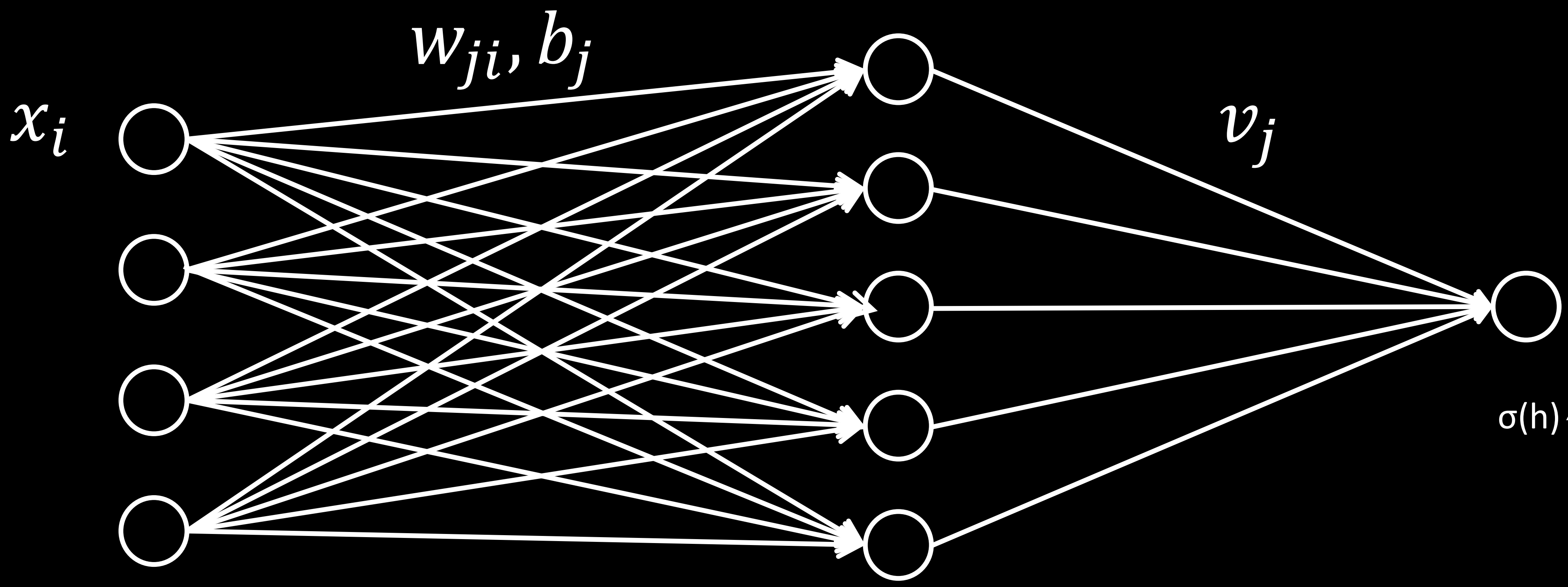
Learning Pseudogap State of HTSC

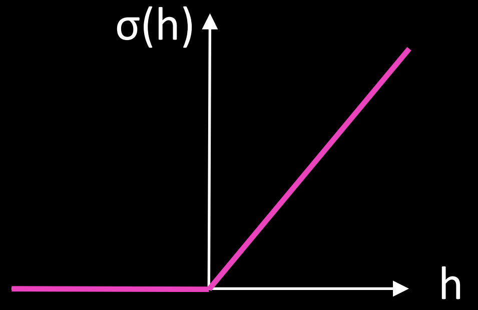


r-space
or
k-space?

The function $h(\vec{x})$?

(Deep) Neural Network (multi-layer perceptron)





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

Local Motif in STS data

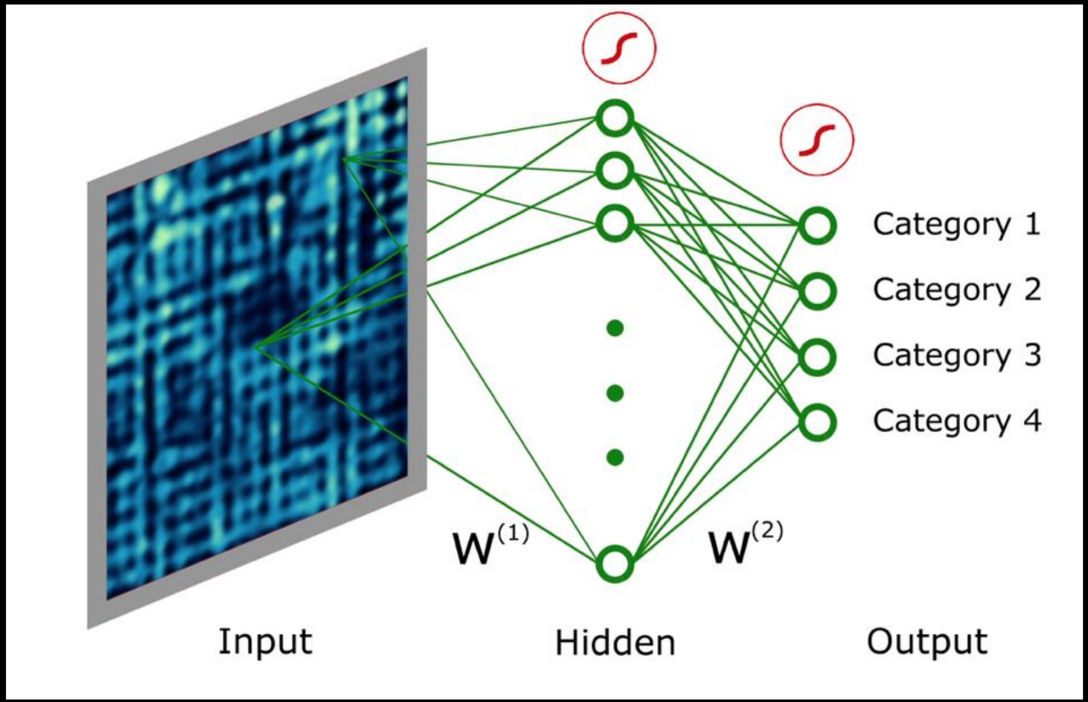
Yi Zhang

Andrej Mesaros

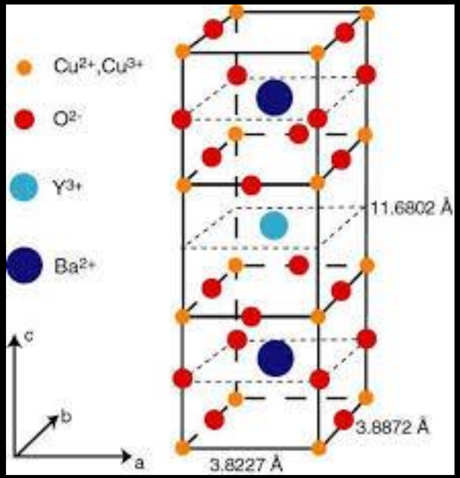
K. Fujita (BNL)

E. Khatami (SJSU)

J.C. Davis
(Oxford/U College Cork)



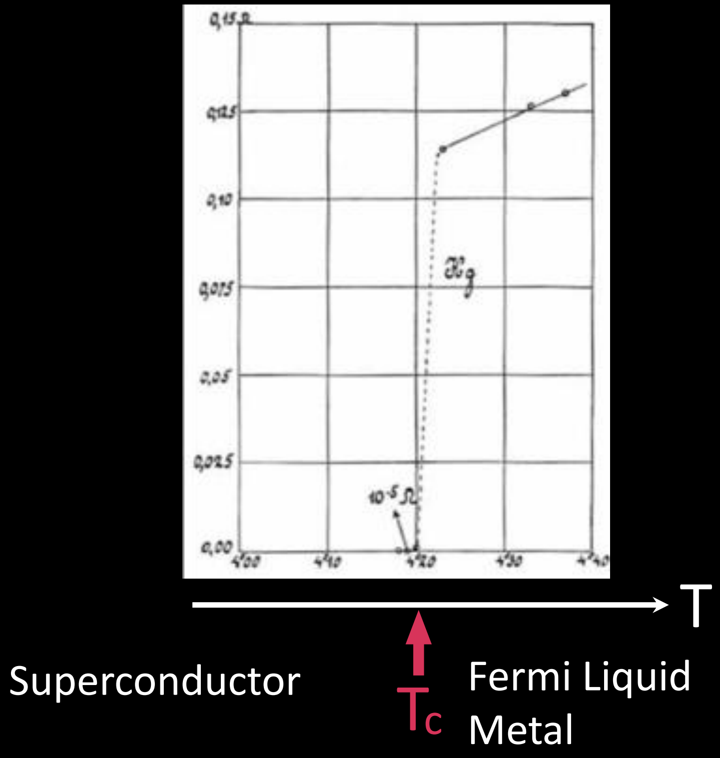
Y. Zhang, A. Mesaros, K. Fujita, J.C. Davis, E. Khatami, EAK et al **arXiv:1808.00479**



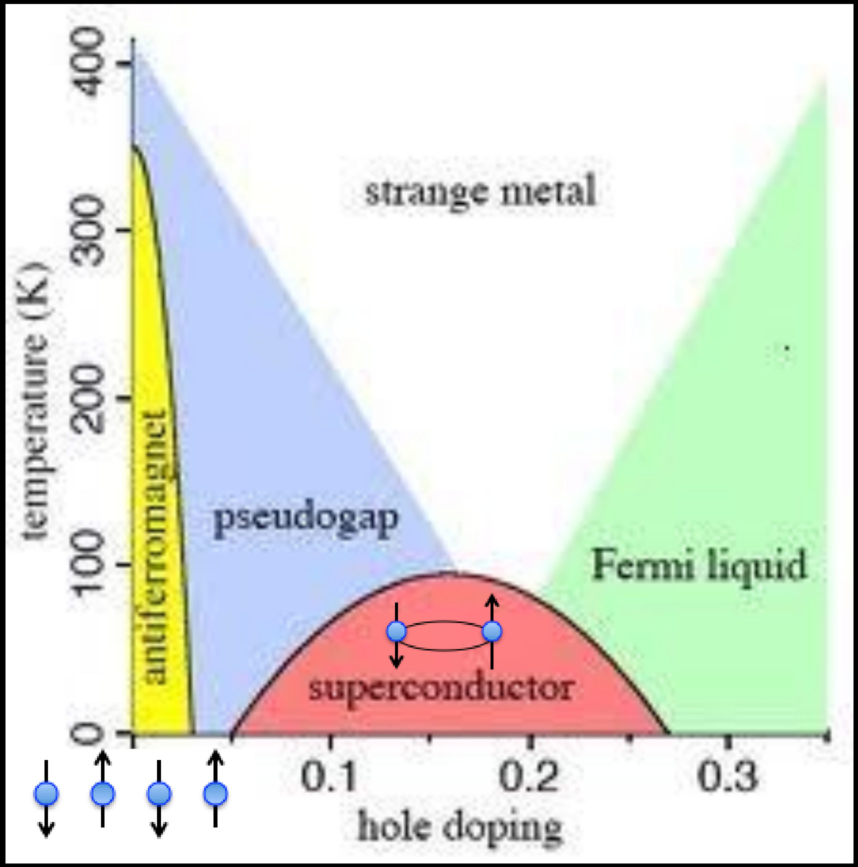
Mysteries of HTSC

The Complex Phase Diagram

Simple PD of conventional SC



Complex PD of high T_c SC



- Multiple "phases"
- Unidentifiable regions

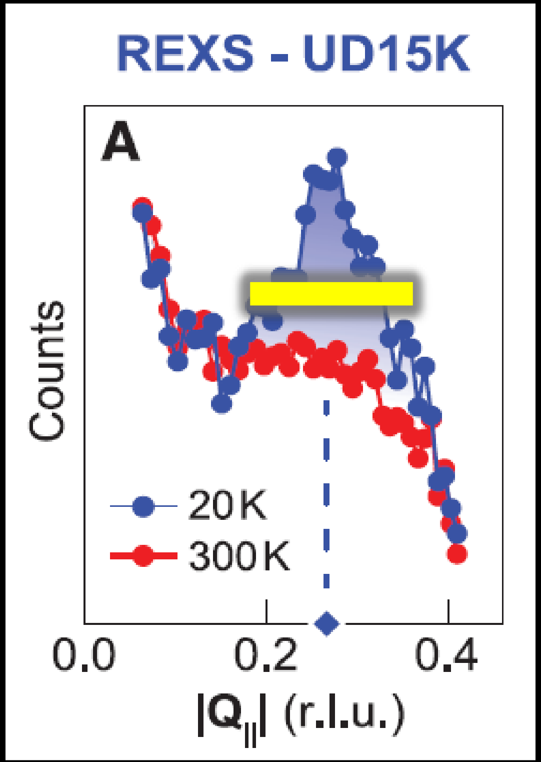
Density Wave and Nematic Order

Hoffman et al, Science (2002)
Howald et al, PRB (2003)
Abbamonte et al , Nature Phys (2005)
Hinkov et al, Science (2008)
Daou et al, Nature (2010)
Lawler et al, Nature (2010)
Ghiringhelli et al, Science (2012)
Blackburn et al PRL (2013)
Comin et al, Science (2014)
de Silva Neto et al, Science (2014)
Fujita et al, PNAS (2014)
Wu et al , Nat. Comm (2015)
Achkar et al, Science (2016)

Density Wave and Nematic

Glassy Order

Hoffman et al, Science (2002)
Howald et al, PRB (2003)
Abbamonte et al , Nature Phys (2005)
Hinkov et al, Science (2008)
Daou et al, Nature (2010)
Lawler et al, Nature (2010)
Ghiringhelli et al, Science (2012)
Blackburn et al PRL (2013)
Comin et al, Science (2014)
de Silva Neto et al, Science (2014)
Fujita et al, PNAS (2014)
Wu et al , Nat. Comm (2015)
Achkar et al, Science (2016)



Comin *et al.* (2014)

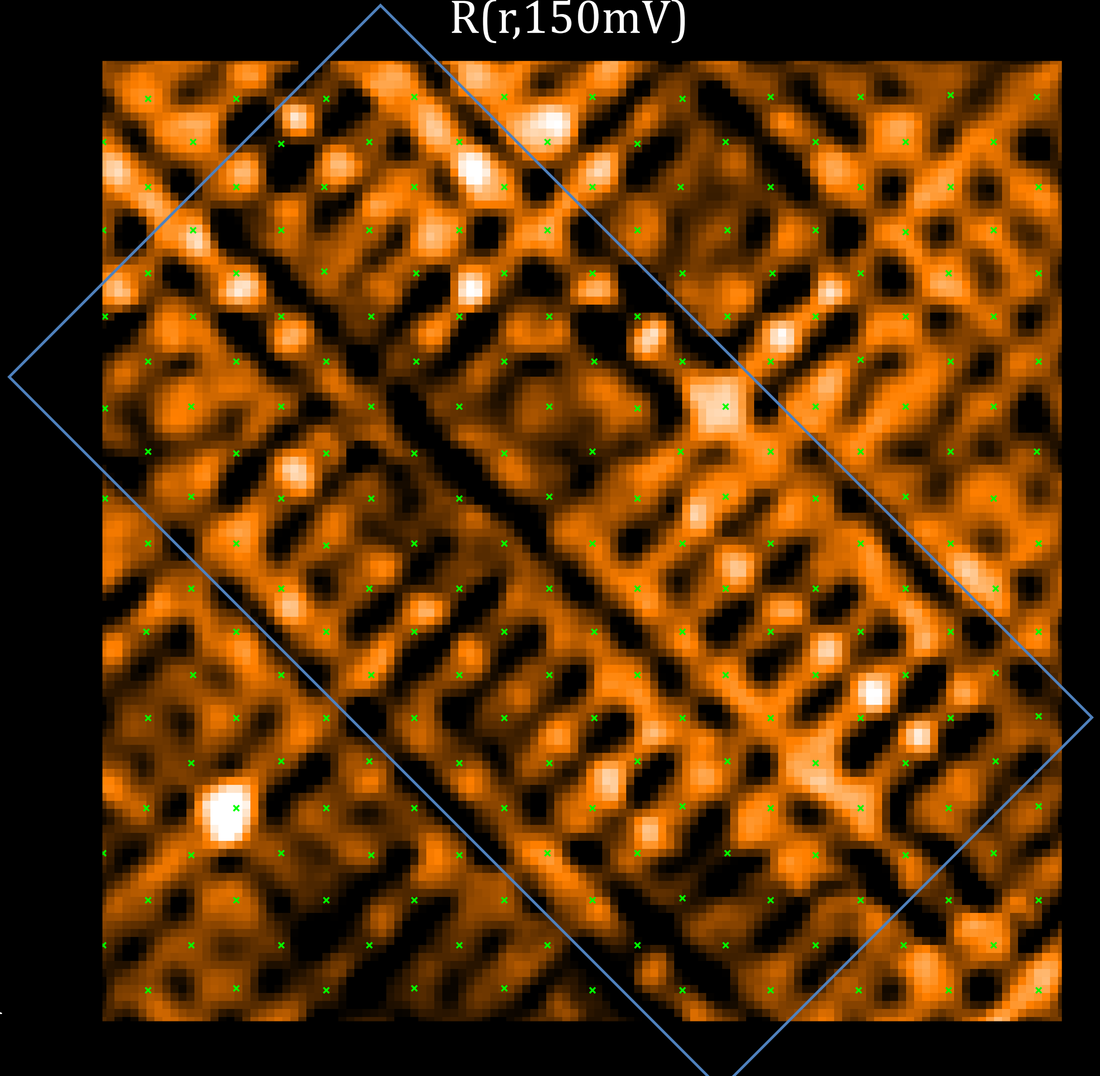
Density Wave and Nematic

Glassy Order

Hoffman et al, Science (2002)
Howald et al, PRB (2003)
Abbamonte et al , Nature Phys (2005)
Hinkov et al, Science (2008)
Daou et al, Nature (2010)
Lawler et al, Nature (2010)
Ghiringhelli et al, Science (2012)
Blackburn et al PRL (2013)
Comin et al, Science (2014)
de Silva Neto et al, Science (2014)
Fujita et al, PNAS (2014)
Wu et al , Nat. Comm (2015)
Achkar et al, Science (2016)

Local Motif!

R(r,150mV)



UD45K
Bi2212 6.2nmx6.2nm

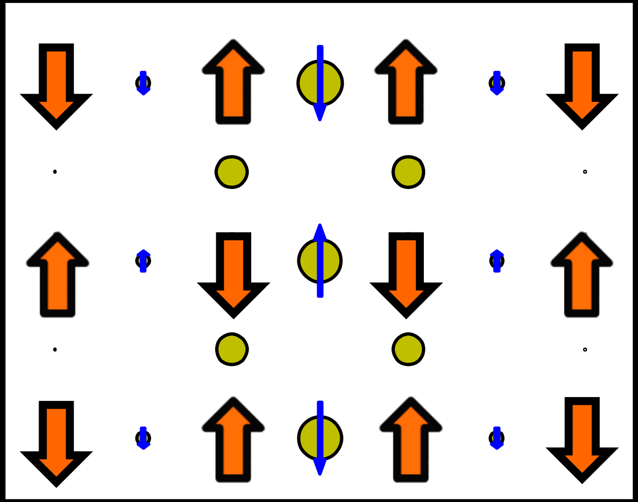
Questions

1. Origin: r-space or k-space?

2. Checkerboard or Stripe?

Strong Coupling Mechanism

- Frustration of AFM order upon doping

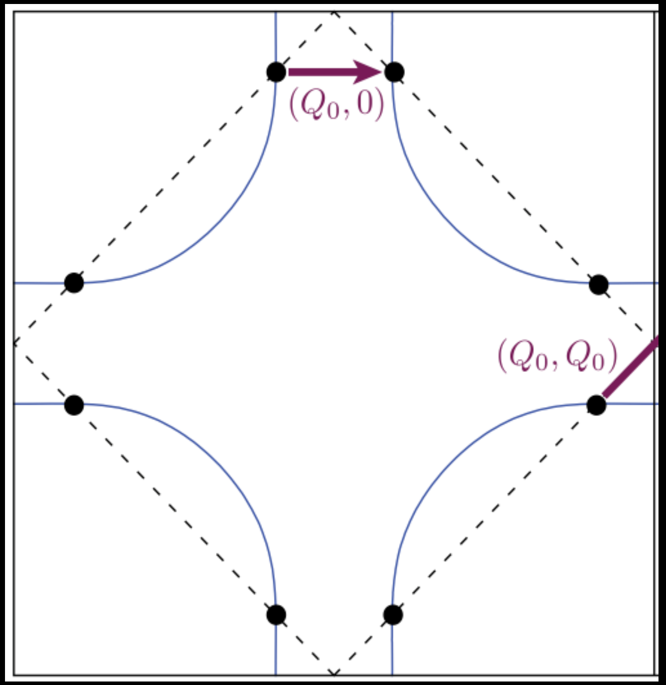


Zaanen, Gunnarson, PRB (1989)
Low, Emery, Fabricious, Kivelson (1994)
Vojta, Sachdev(1999)
White, Scalapino,PRL(1998)
Capponi, Poilblanc (2002)
Corboz, Rice, Troyer, PRL (2014)
Fischer, EAK *et al.*, NJP (2014)

Commensurate Charge Modulation,
λ= 4a at p=1/8

Weak Coupling Mechnism

- Nesting driven Fermi surface instability



Efitov et al, Nature Physics (2013)
Pepin et al, PRB (2014)
Wang, Chubukov, PRB (2014)
Loder et al, PRL (2011)

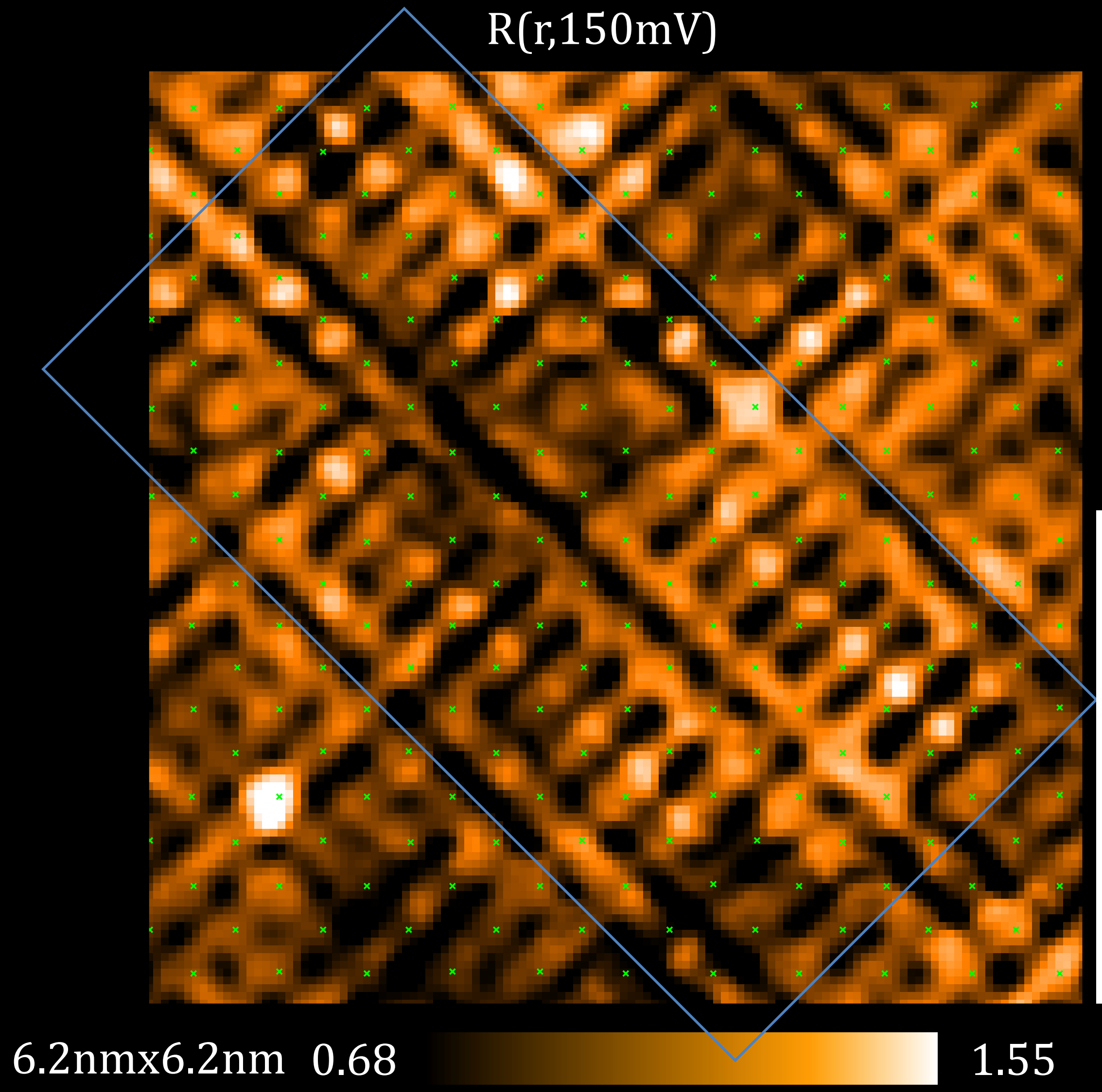
Incommensurate,
Q decrease with p

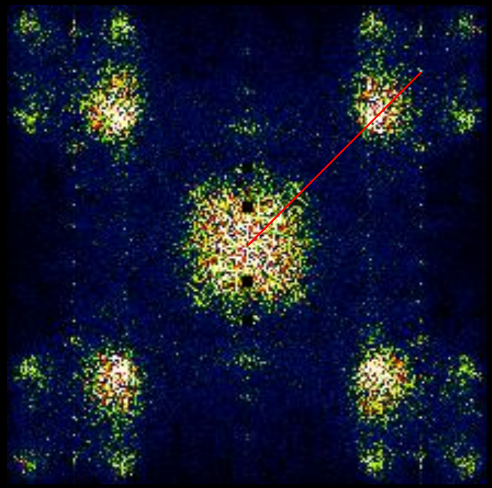
Conventional Approach

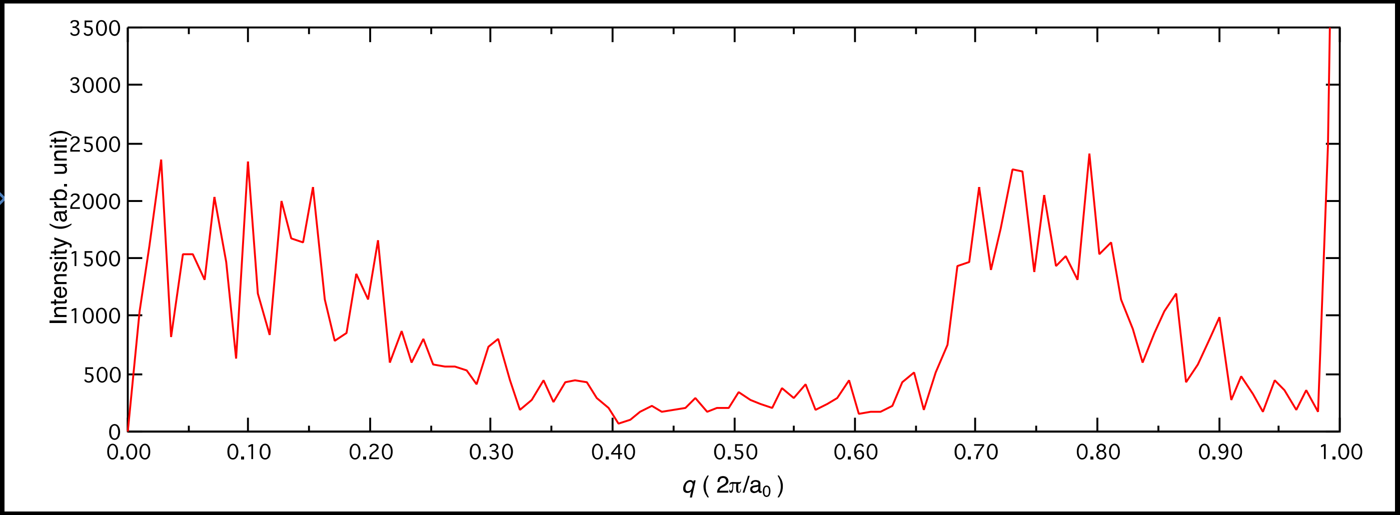
1. Fourier Transfrom

2. Compress FT down to the peak location of a line cut

UD45K
Bi2212



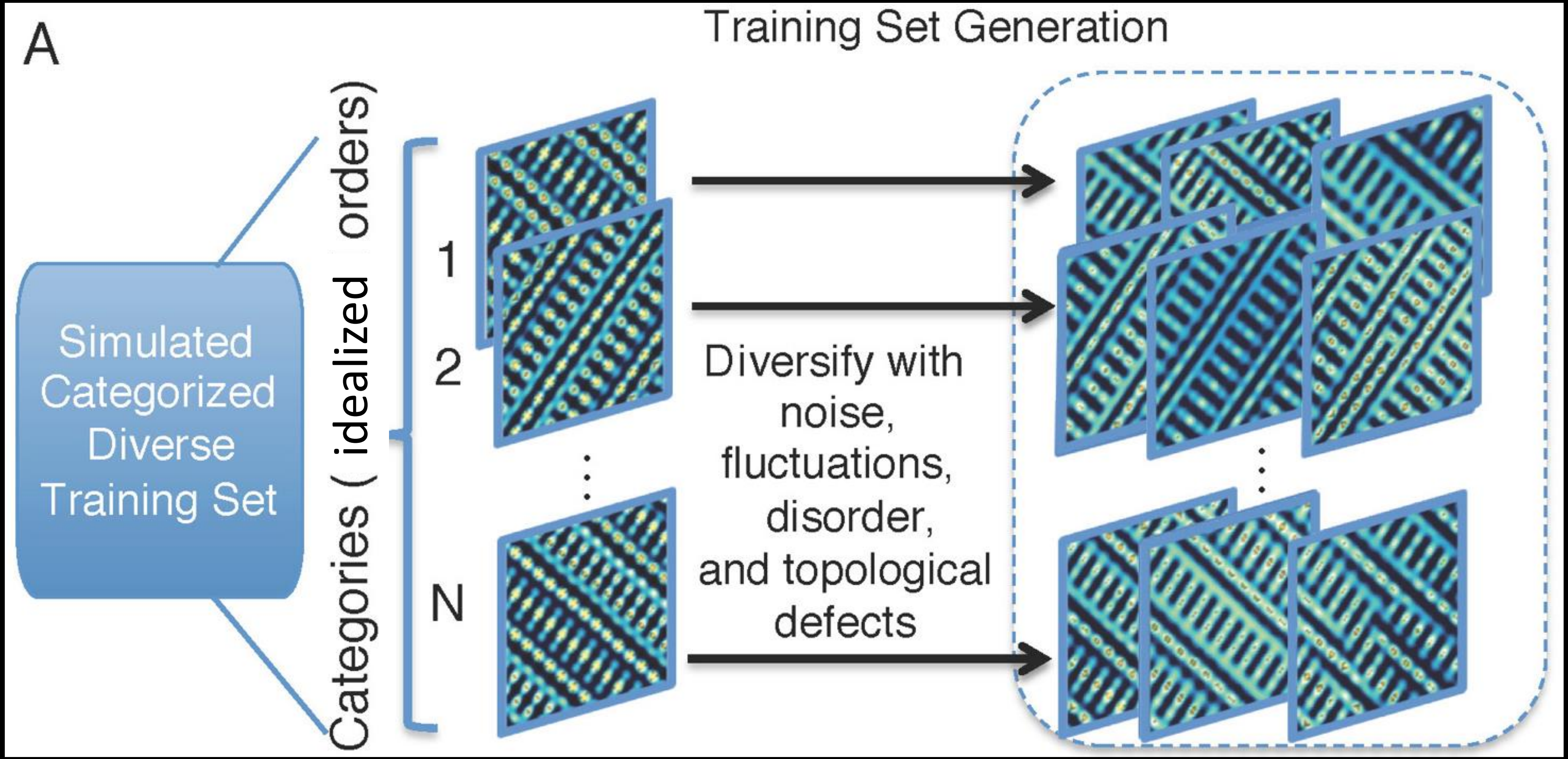




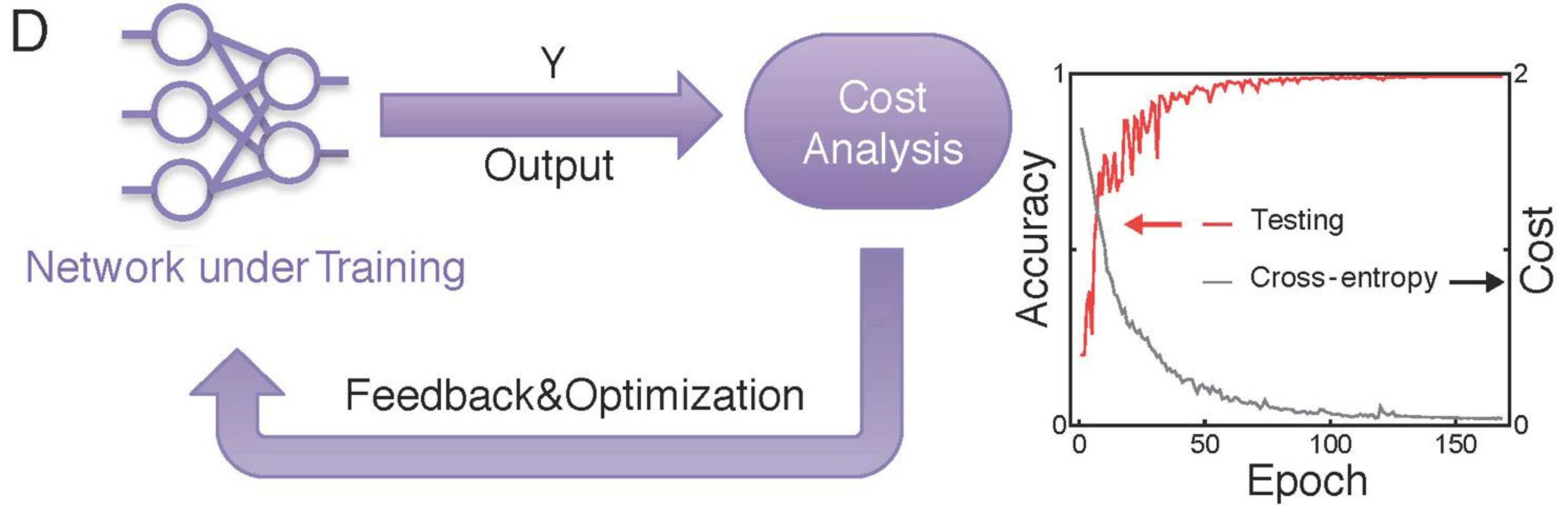
Linecut through (0,0)-(1,0)

Robertson et al (2006),
Del Maestro et al (2006)
declared defeat within manual schemes!

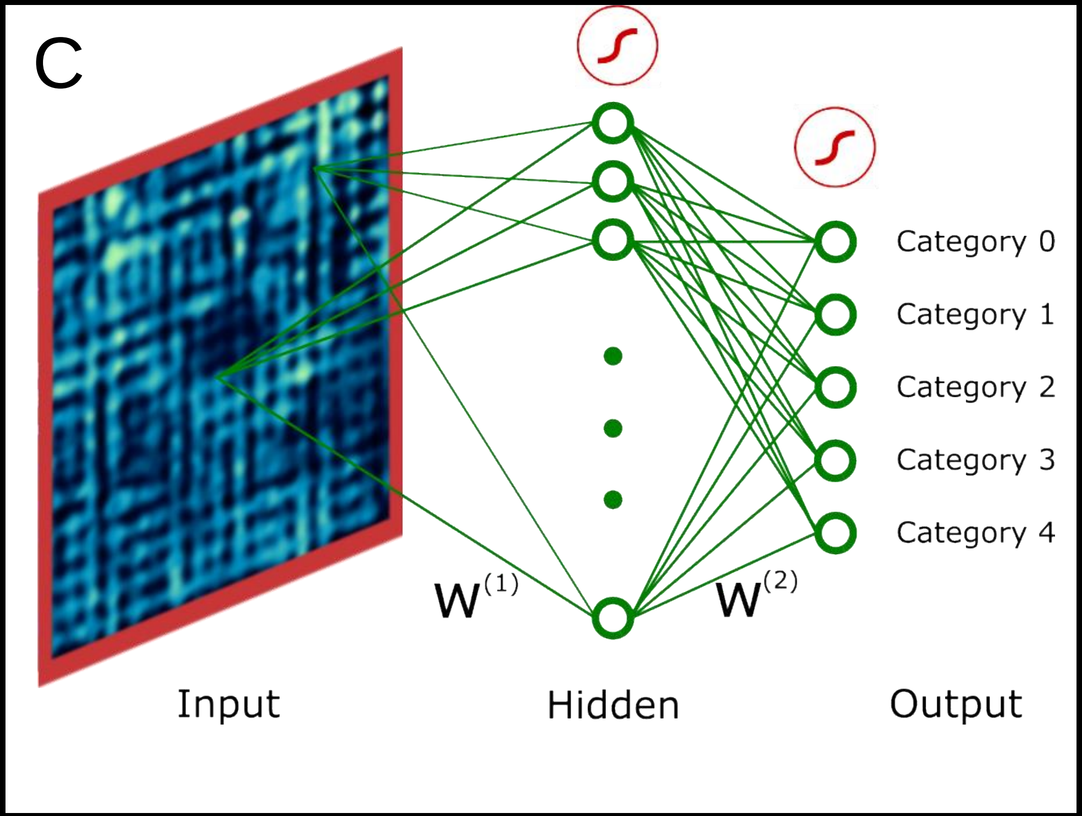
3-stage protocol: I



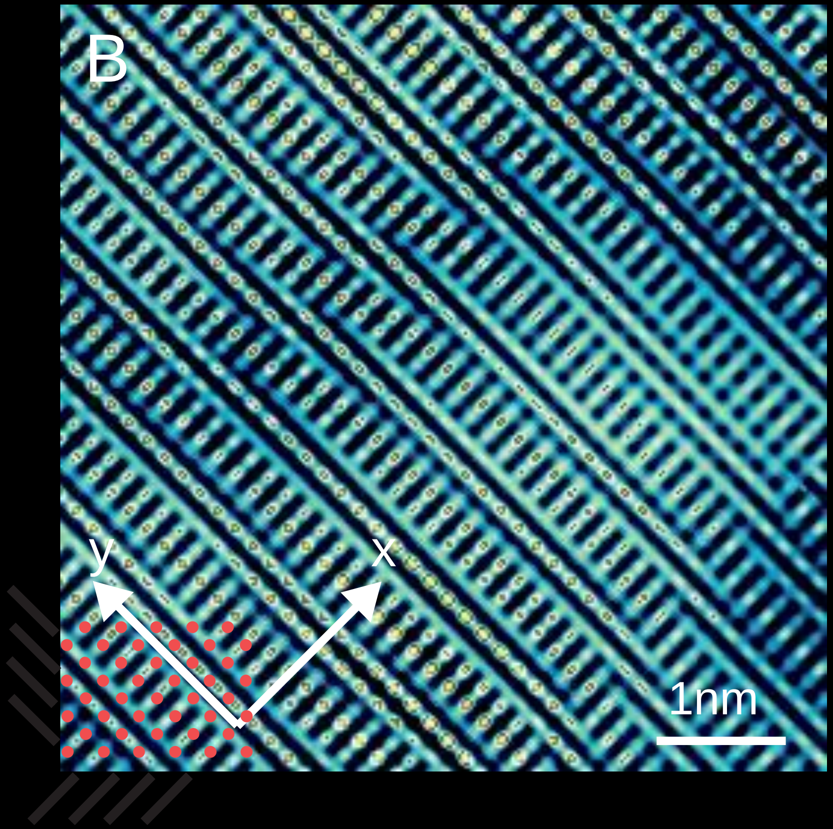
3-stage protocol: II



3-stage protocol: III



Training Set Generation

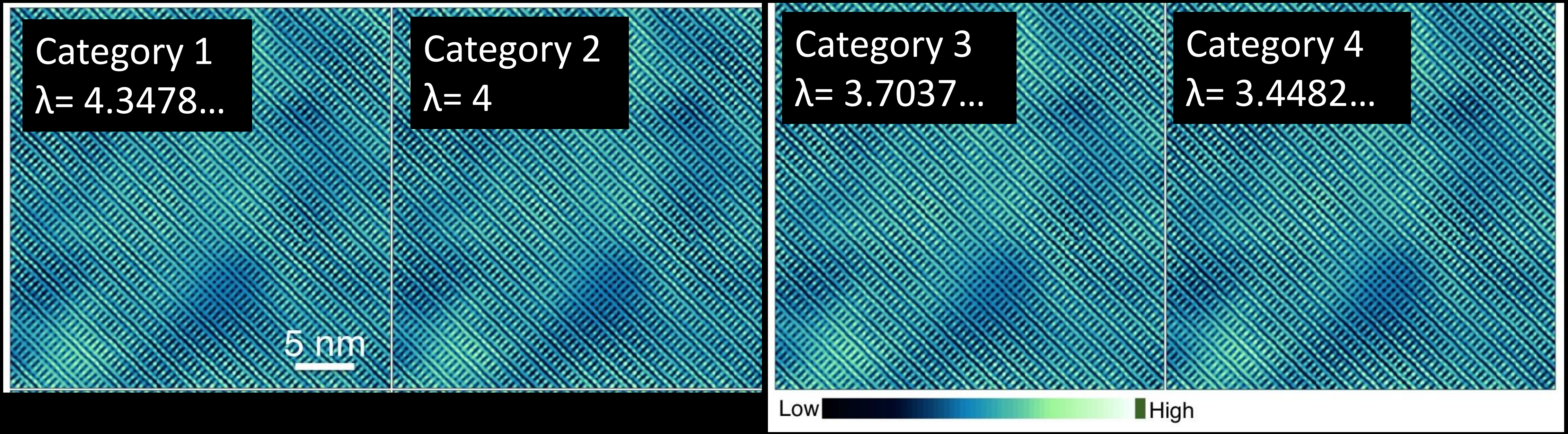


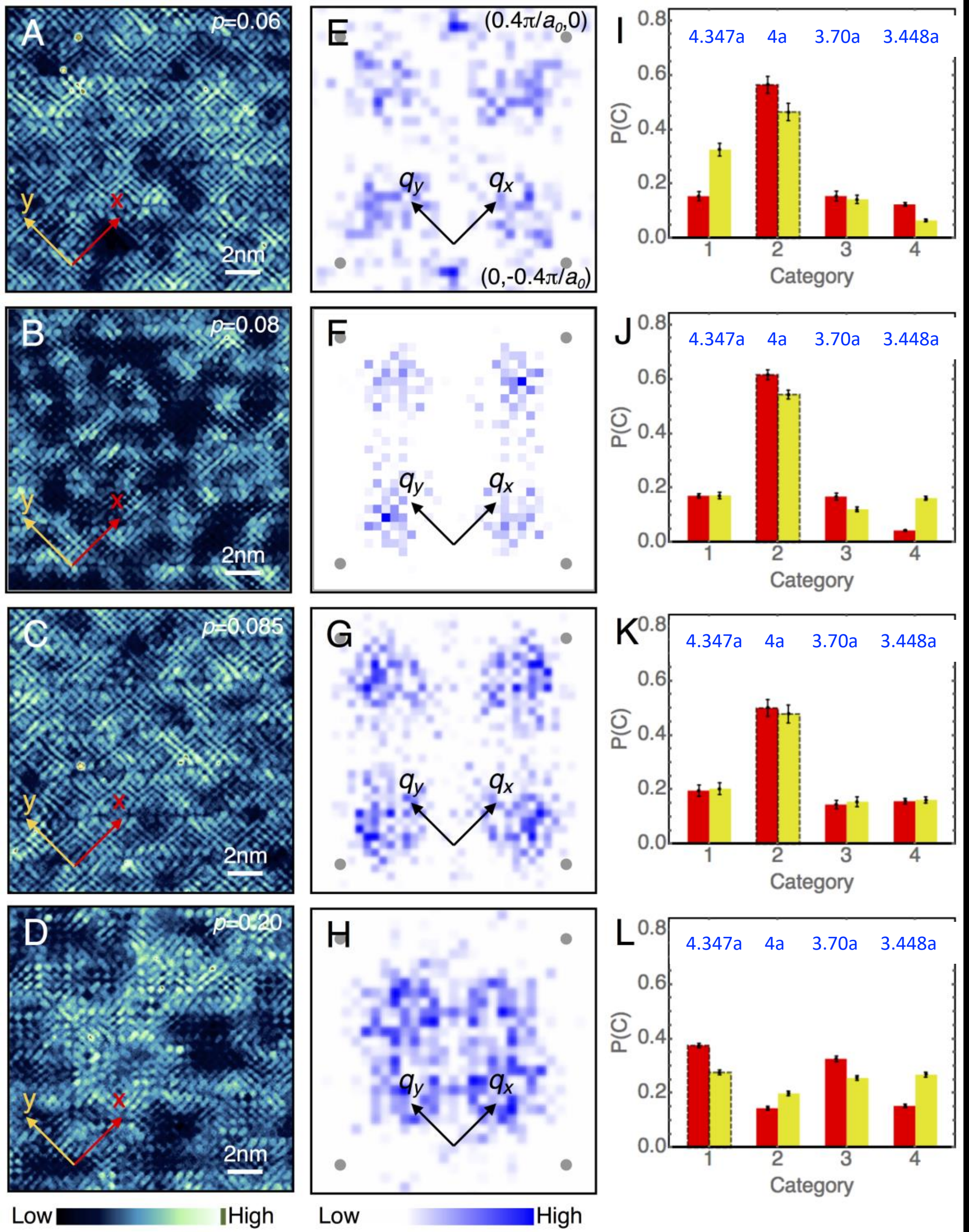
$$A_d(\boldsymbol{x}) = \prod_{i=1}^{n_d} (1 - exp(-|\boldsymbol{x} - \boldsymbol{x}_i|/\xi_d))$$

$$\varphi_d(x,y) = \sum_{j=1}^{n_d} Arg\left[sgn(w_j)(x - x_j) + i(y - y_j)\right],$$

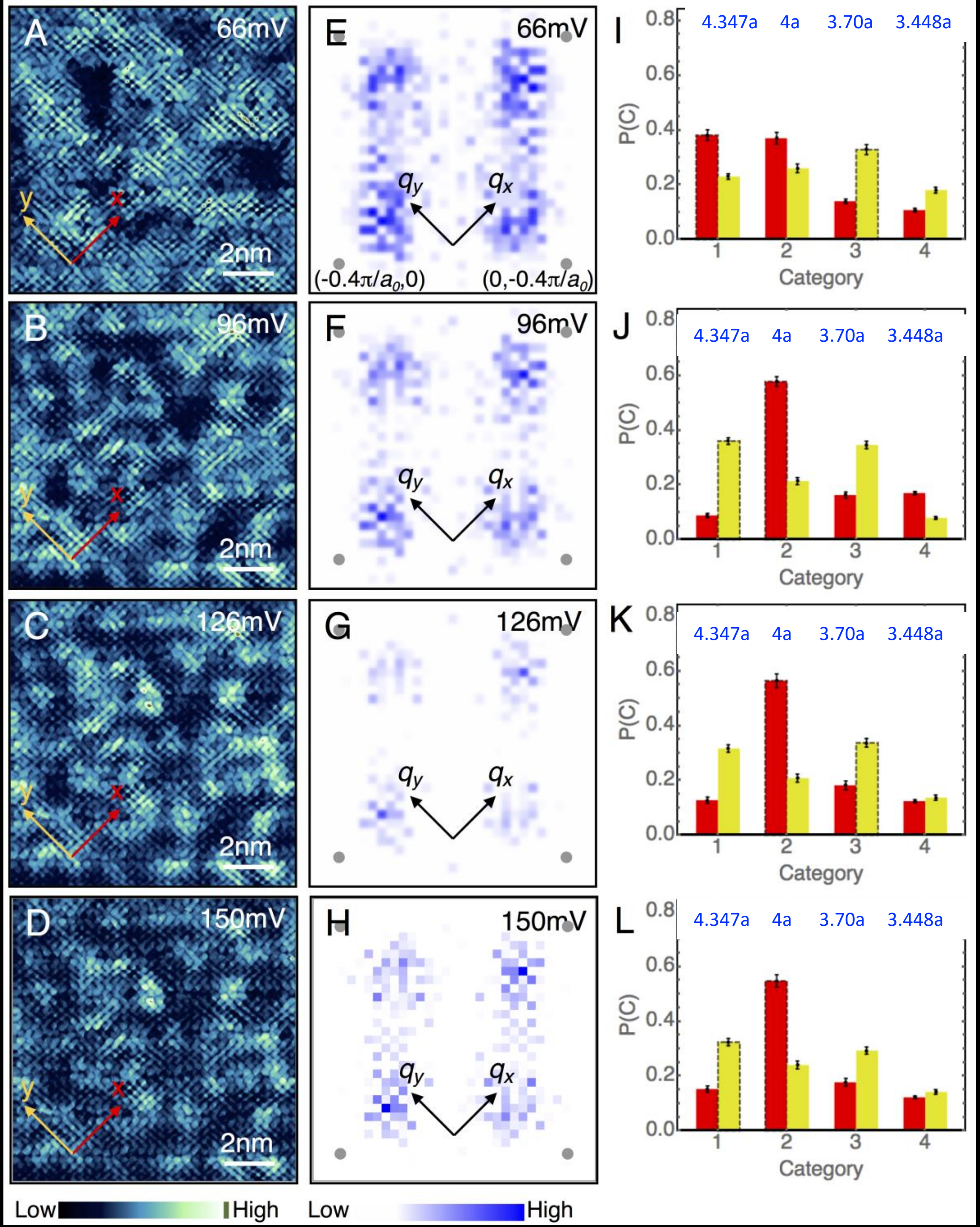
$$I_{C,f,d}^{DFF}(x,y) = A_{DFF}\left[1 + \varepsilon_A\, A_f(x,y)\right] A_d(x,y)\, Cos\left(Q_C x + \varepsilon_\varphi \varphi_f(x,y) + \varphi_d(x,y) + \varphi_{DFF}\right).$$

Four Candidate Wave Vectors

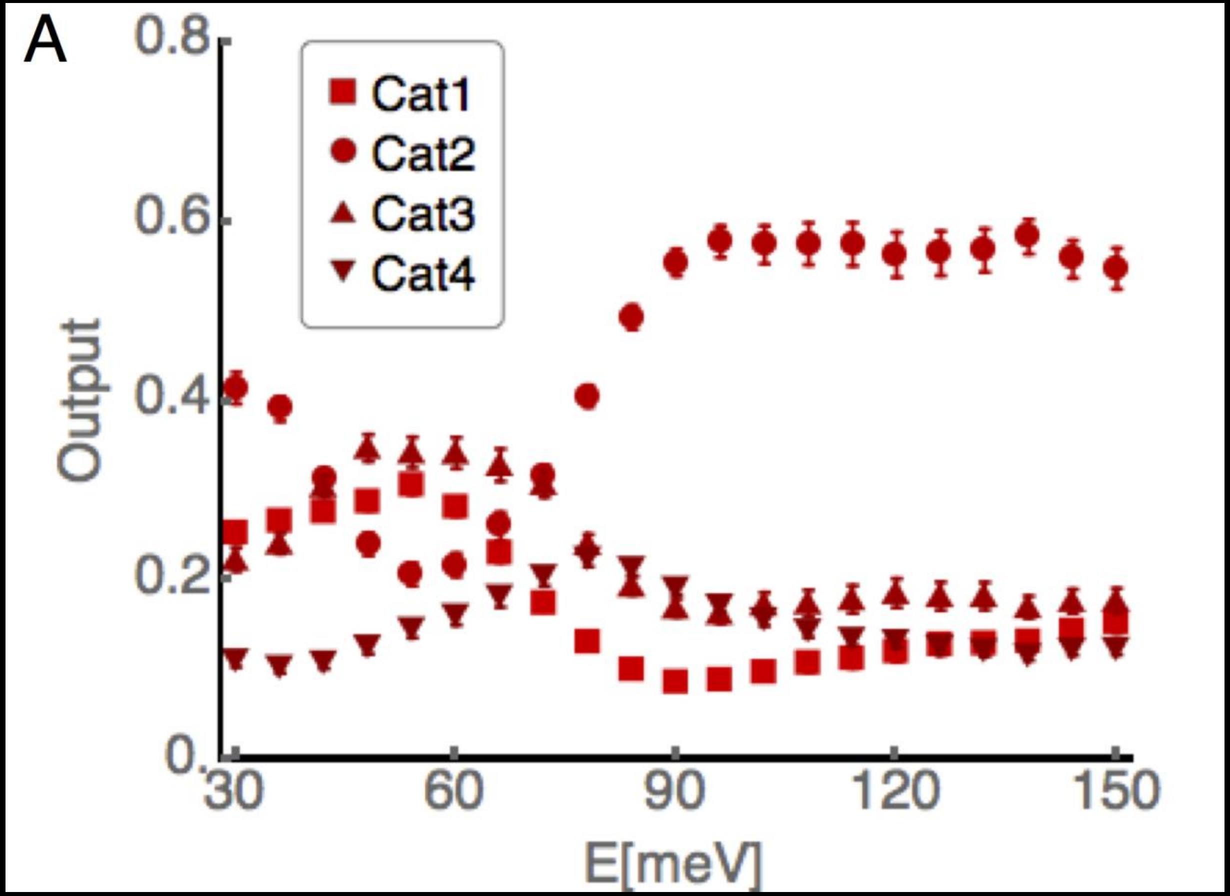




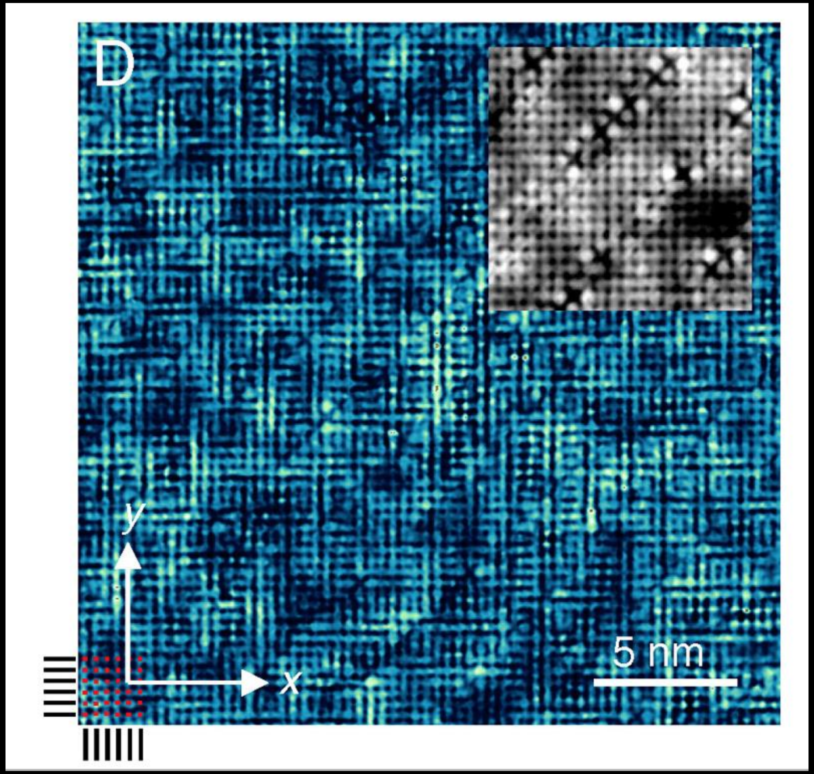
Doping Dependence

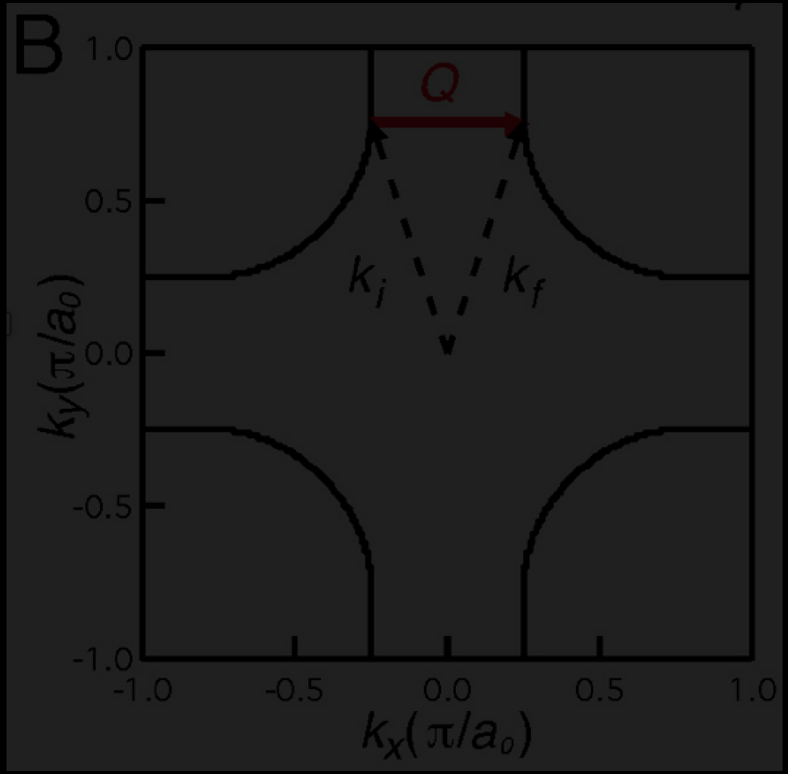


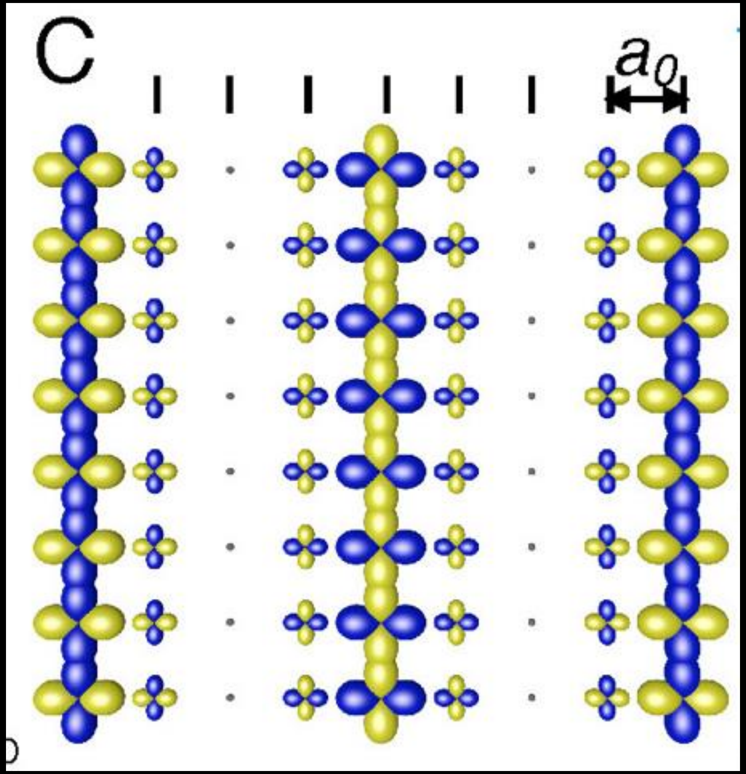
Energy Dependence



Hypothesis test







Unidirectional, lattice commensurate, period 4 charge modulations.

Unsupervised ML of Diffuse Scattering (X-ray)

Golden Needle in Hay Stacks: X-ray Diffuse Scattering

Jordan Venderley

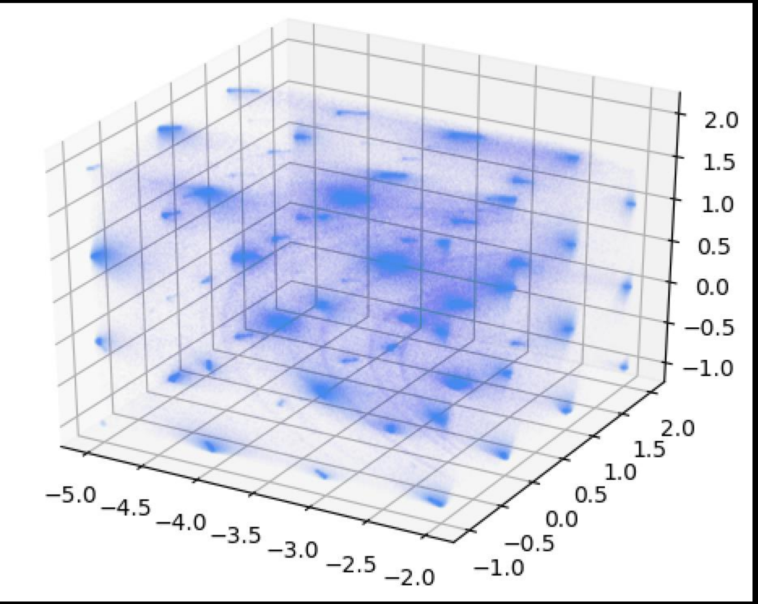
Mike Matty

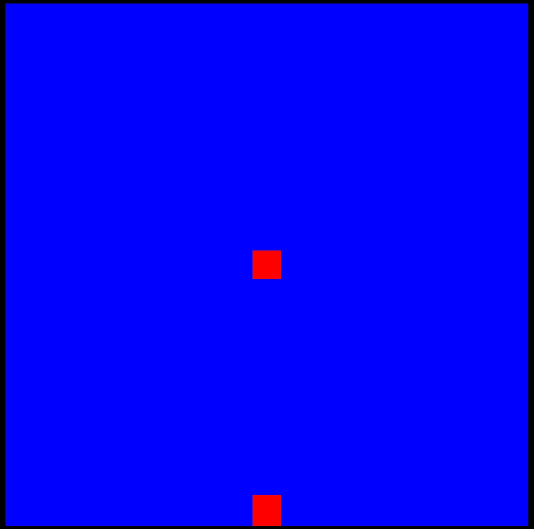
Geoff Pleiss
(Cornell, CS)

Jacob Ruff
(CHESS)

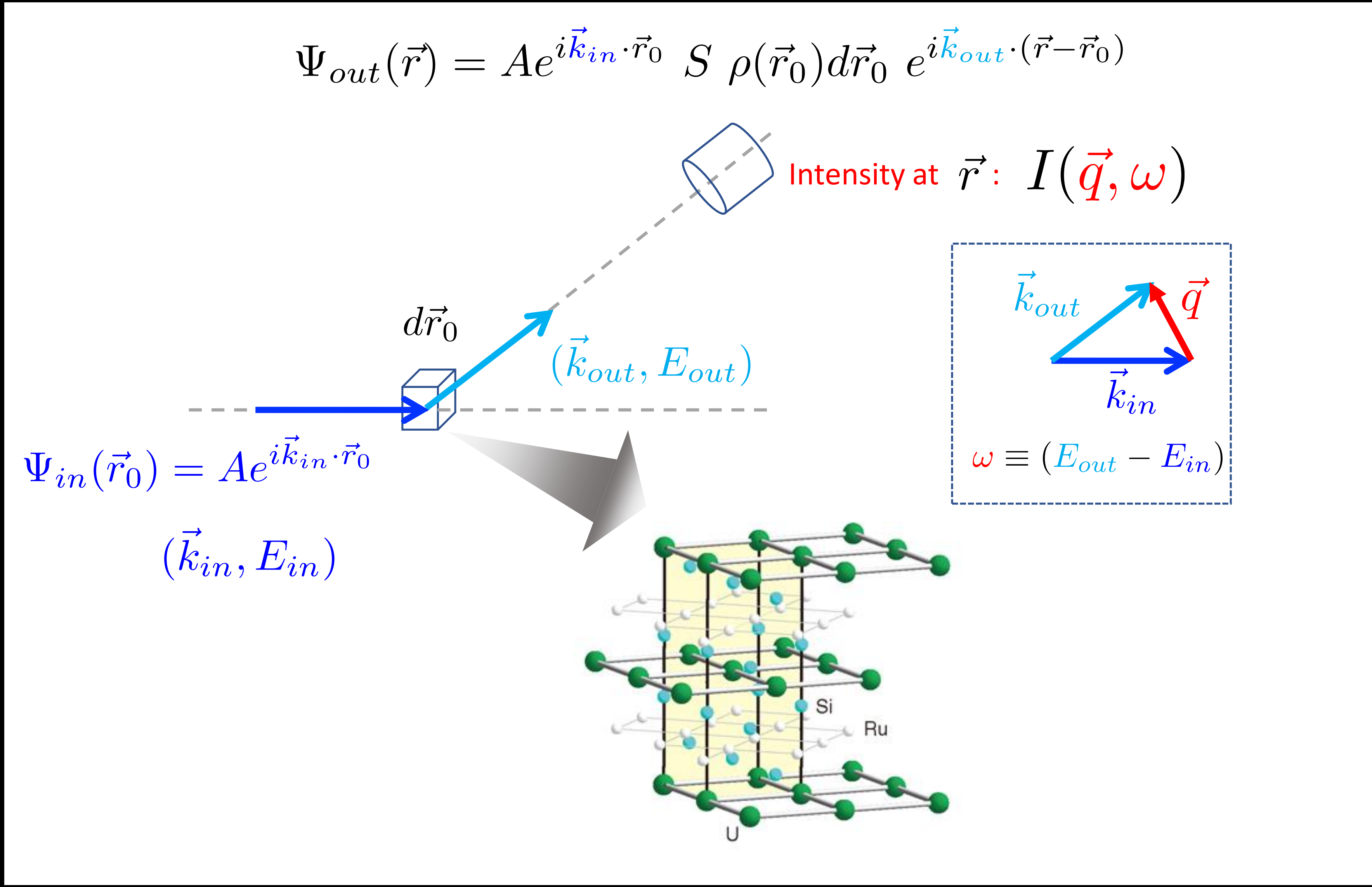
K. Winberger
(Cornell, CS)

A. Wilson
(Cornell, ORIE)





What do we measure?



What do we measure?

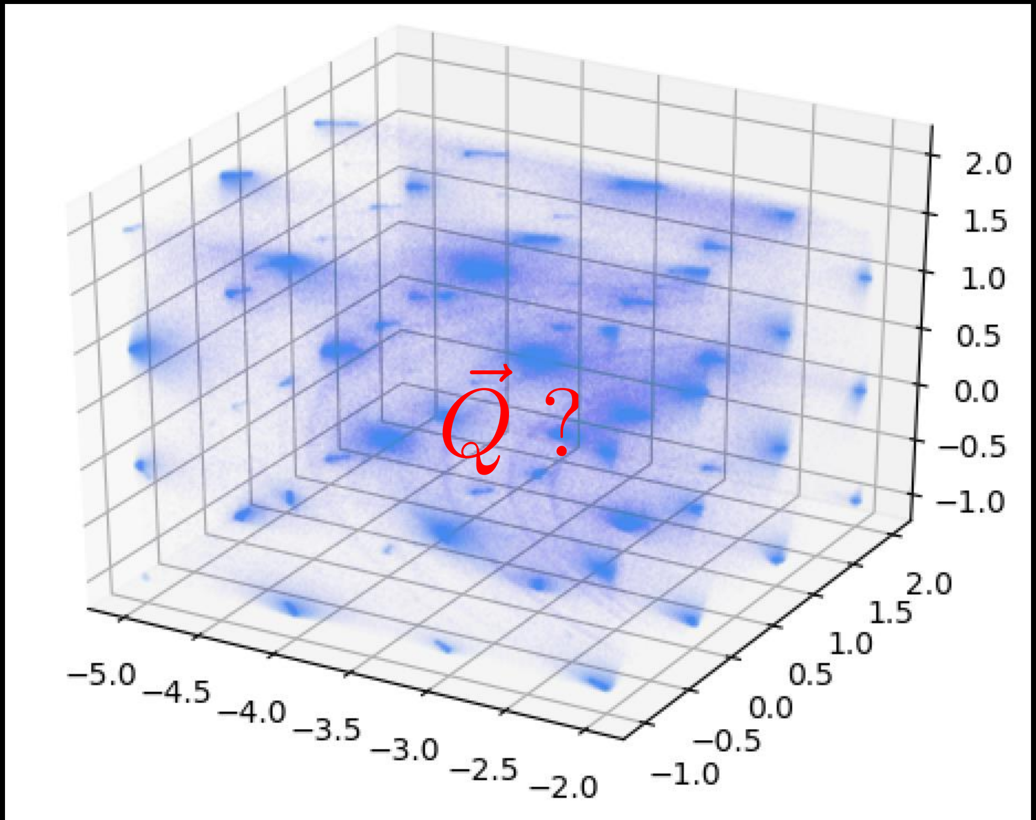
$$\Psi_{out}^{tot} \propto \int d\vec{r}_0 \; e^{i\vec{k}_{in}\cdot\vec{r}_0} \rho(\vec{r}_0) e^{i\vec{k}_{out}\cdot(\vec{r}-\vec{r}_0)} = \; e^{i\vec{k}_{out}\cdot\vec{r}} \; \widetilde{\rho}(\vec{q})$$

- $I(\vec{q};T) \propto |\widetilde{\rho}(\vec{q};T)|^2$: Fourier amplitude of density
- Density Wave with wave vector $\vec{Q}$

$$\rho(\vec{r};T) = \rho_0 + \mathrm{Re}\left[\Delta_{\vec{Q}}(T)\; e^{i\vec{Q}\cdot\vec{r}}\right]$$

- $I(\vec{Q};T) \propto |\Delta_{\vec{Q}}(T)|^2$: the Order Parameter

Data-driven challenges in Reciprocal Space



(T)

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

A Traditional Generative Model

- Ginzburg-Landau Theory: $\Delta_{\vec{Q}}(T;\{r,s\}) = \sqrt{\frac{r(T-T_c)}{s}}$

- Training Data

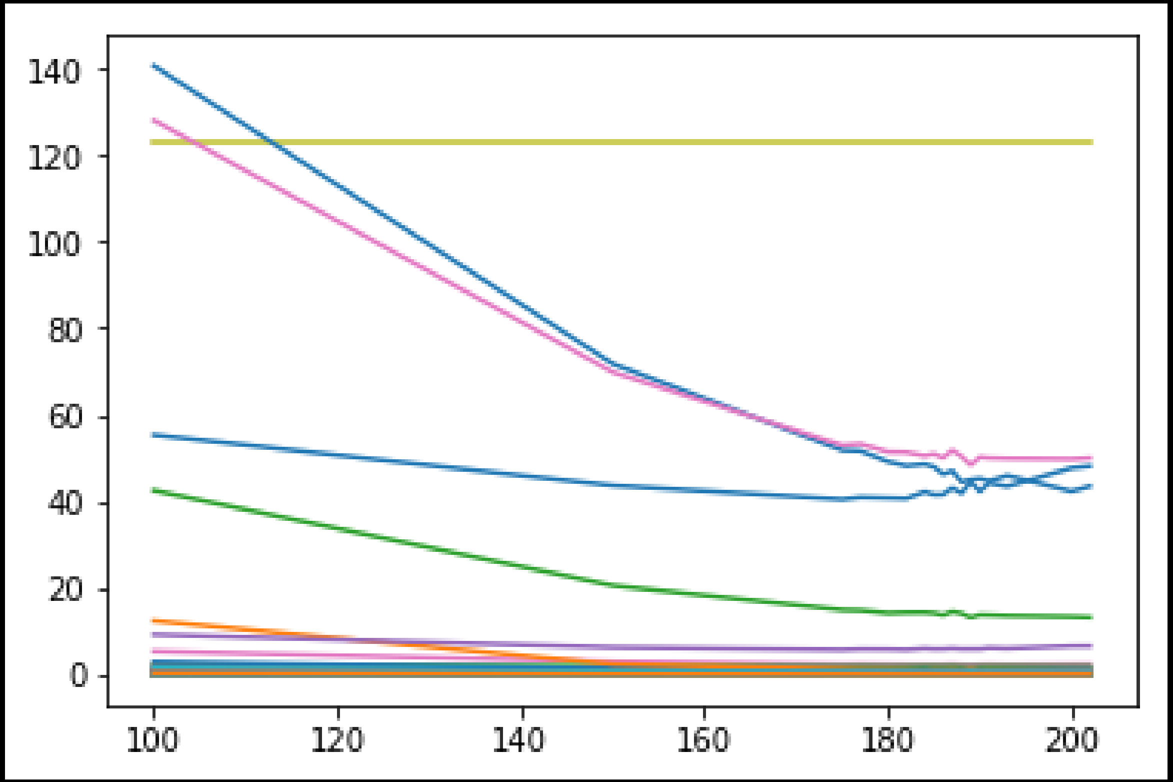
$$\mathbb{T} \equiv \{T_1, T_2, \cdots, T_m\}$$
$$\mathbf{\Delta} \equiv \{\Delta_1, \Delta_2, \cdots, \Delta_m\}$$

Regression → $\{r^*, s^*\}$

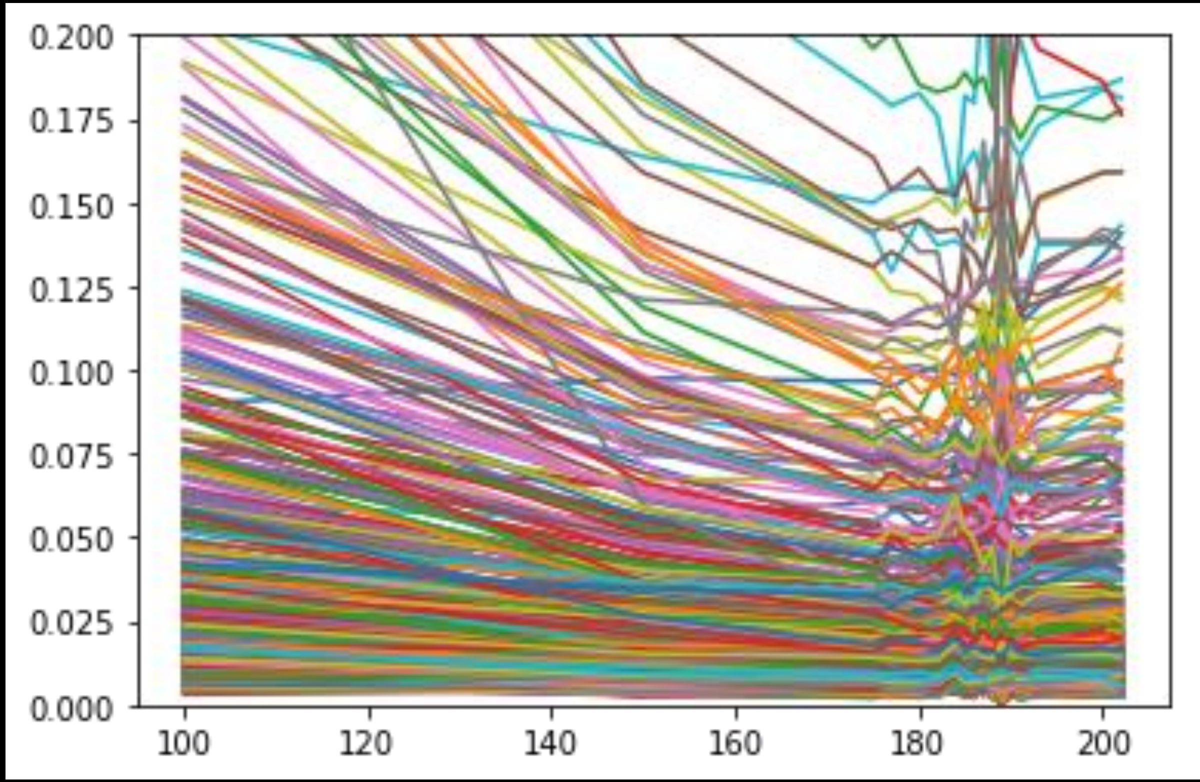
- Prediction given testing points $\mathbb{T}^* \equiv \{T_1^*, T_2^*, \cdots, T_n^*\}$

$$\mathbf{\Delta}^* = \{\Delta(T_i^*; r^*, s^*)\}_{i=1,\cdots,n}$$

What if



140
120
100
80
60
40
20
0
100
120
140
160
180
200



0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
100
120
140
160
180
200

Gaussian Process Mixture Model

- Learn the distribution over functions that capture

  $I(\vec{q}_i, T_l)$ and $i = 1, \cdots, N^3$, and $l = 1, \cdots, m$

- Predictive Posterior Distribution

$$p(\mathbf{y}^*|\mathbf{x}^*, \{\mathbf{y}, \mathbf{X}\}, \{\pi, \mu, \mathbf{\Sigma}\}) = \sum_{k=1}^{K} \pi_k(x^*) GP(\mu_k(\mathbf{x}^*), \Sigma_k(\mathbf{x}^*))$$

Learned weight

$$p(\mathbf{y}^*|\mathbf{x}^*, \{\mathbf{y}, \mathbf{X}\}, \{\pi, \mu, \mathbf{\Sigma}\}) = \sum_{k=1}^{K} \underbrace{\pi_k(x^*)}_{\text{Learned weight}} GP(\mu_k(\mathbf{x}^*), \Sigma_k(\mathbf{x}^*))$$

Training Set (Exp. Data)

$$\underline{X} = \begin{bmatrix} (\{\vec{q}_i\}, T_1) \\ \vdots \\ (\{\vec{q}_i\}, T_m) \end{bmatrix}$$

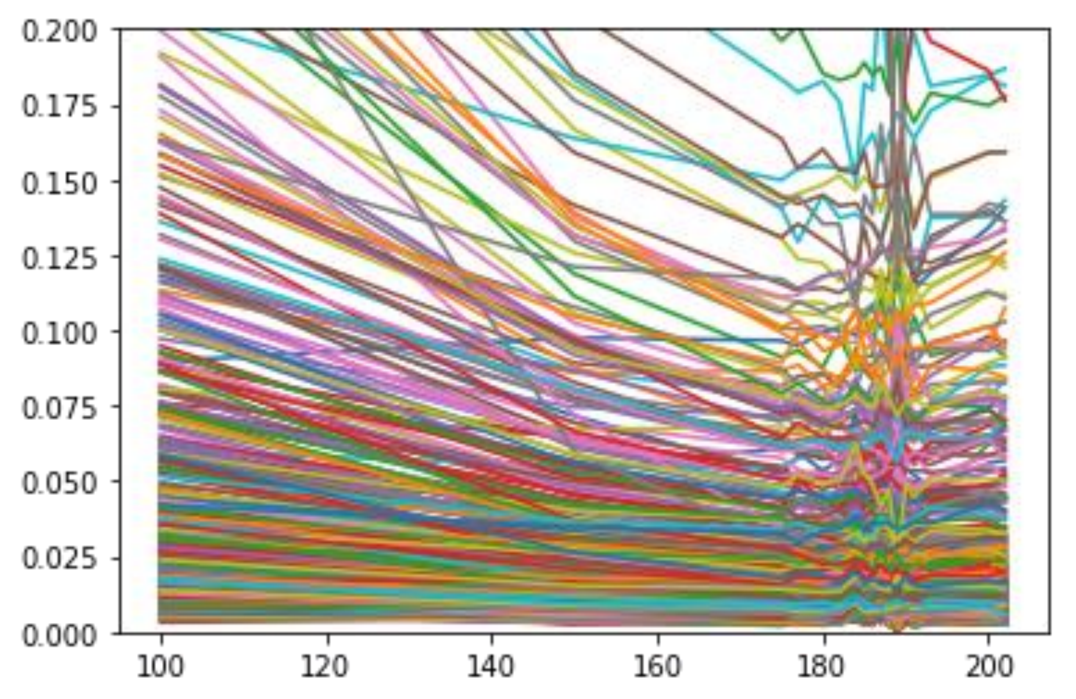
$$y = \begin{bmatrix} \{I(\vec{q}_i, T_1)\} \\ \vdots \\ \{I(\vec{q}_i, T_m)\} \end{bmatrix}$$

Testing Point $x^* = (\vec{q}^*, T^*)$

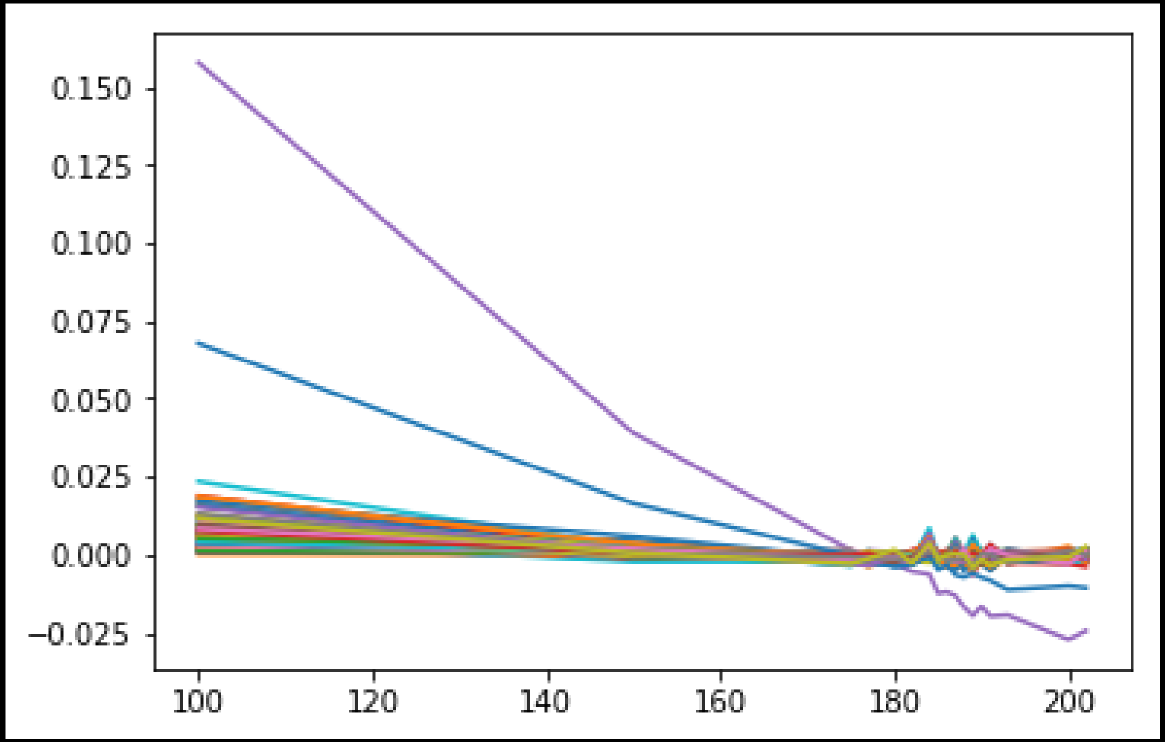
$$f(\cdot) \sim GP(m(\cdot), k(\cdot, \cdot))$$

$$\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_m) \end{bmatrix} \sim N\left(\begin{bmatrix} m(x_1) \\ \vdots \\ m(x_m) \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_m) \\ \vdots & \ddots & \vdots \\ k(x_m, x_1) & \cdots & k(x_m, x_m) \end{bmatrix} \right)$$

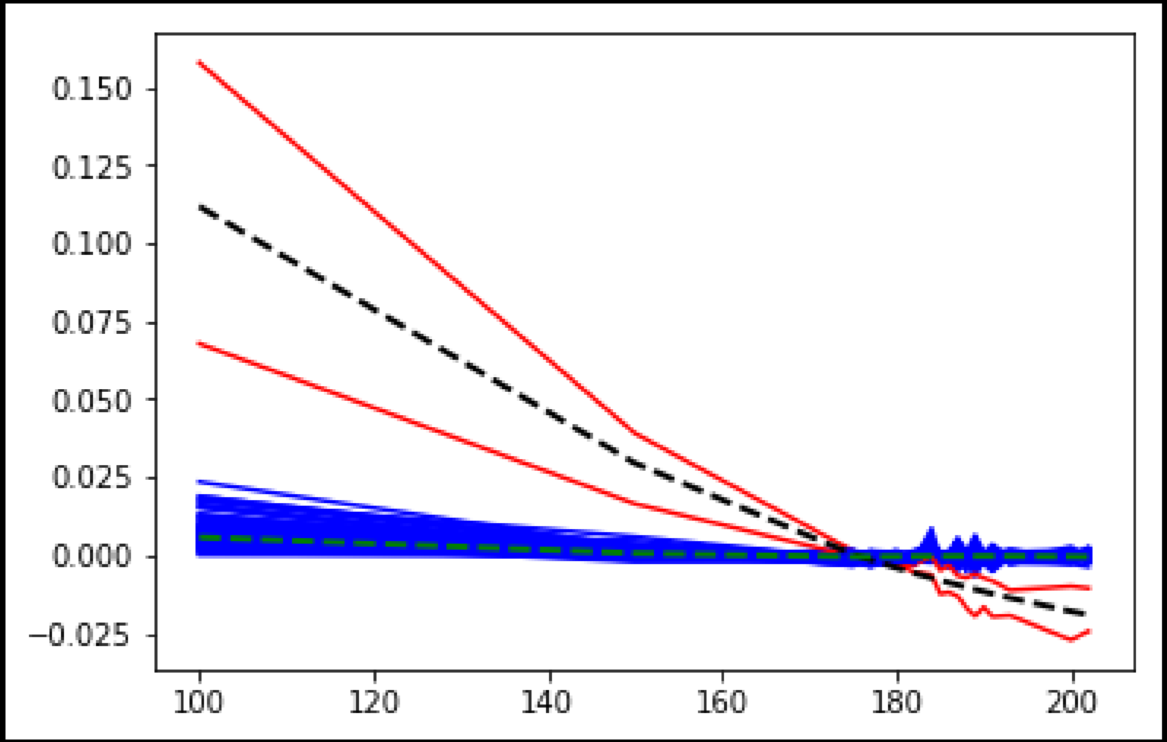
Results


0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
100
120
140
160
180
200

Results

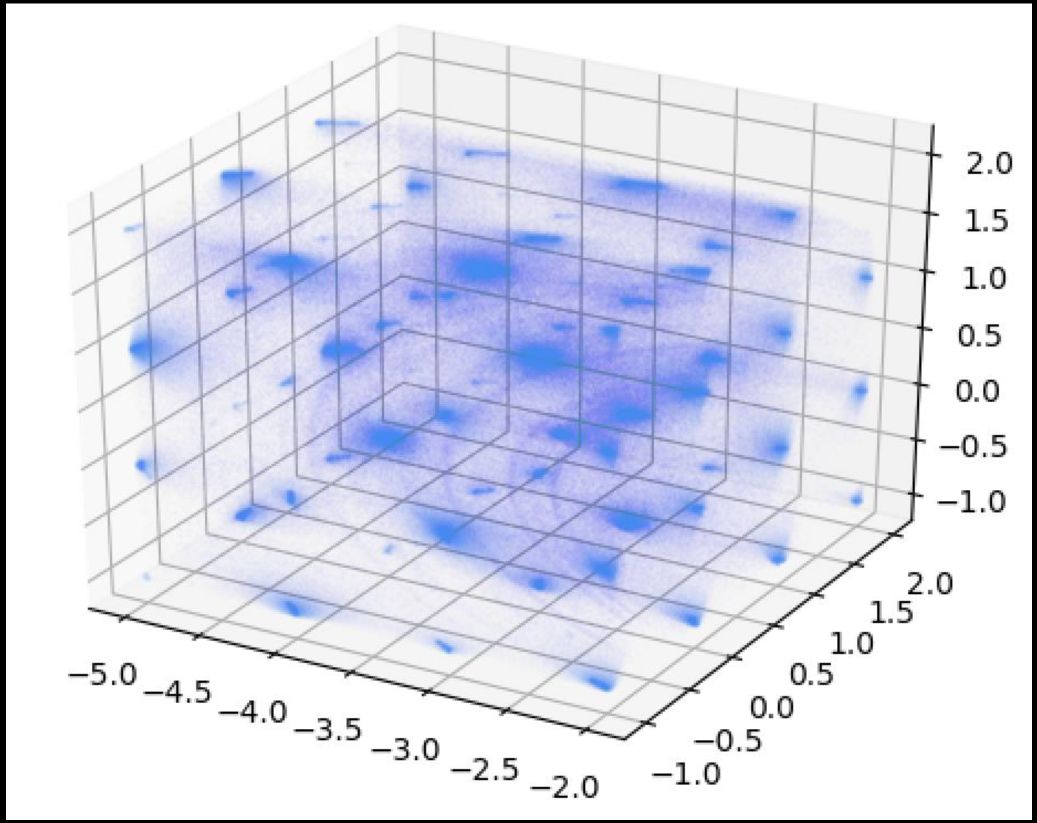


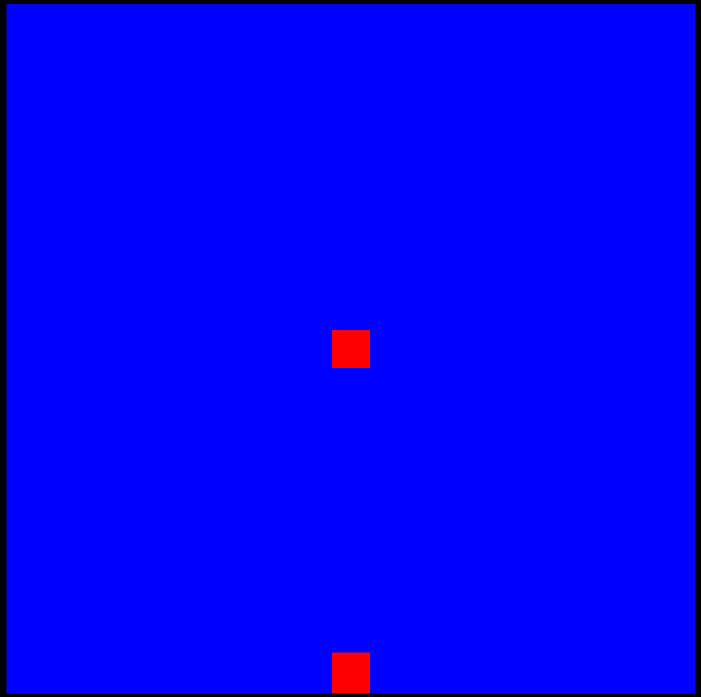
0.150
0.125
0.100
0.075
0.050
0.025
0.000
−0.025
100
120
140
160
180
200



0.150
0.125
0.100
0.075
0.050
0.025
0.000
−0.025
100
120
140
160
180
200

Results





Machine Learning Quantum Emergence

The journey has just begun….

- Supervised ML: Hypothesis test, OP symmetry

- Unsupervised ML: Clustering in Reciprocal space

FIN