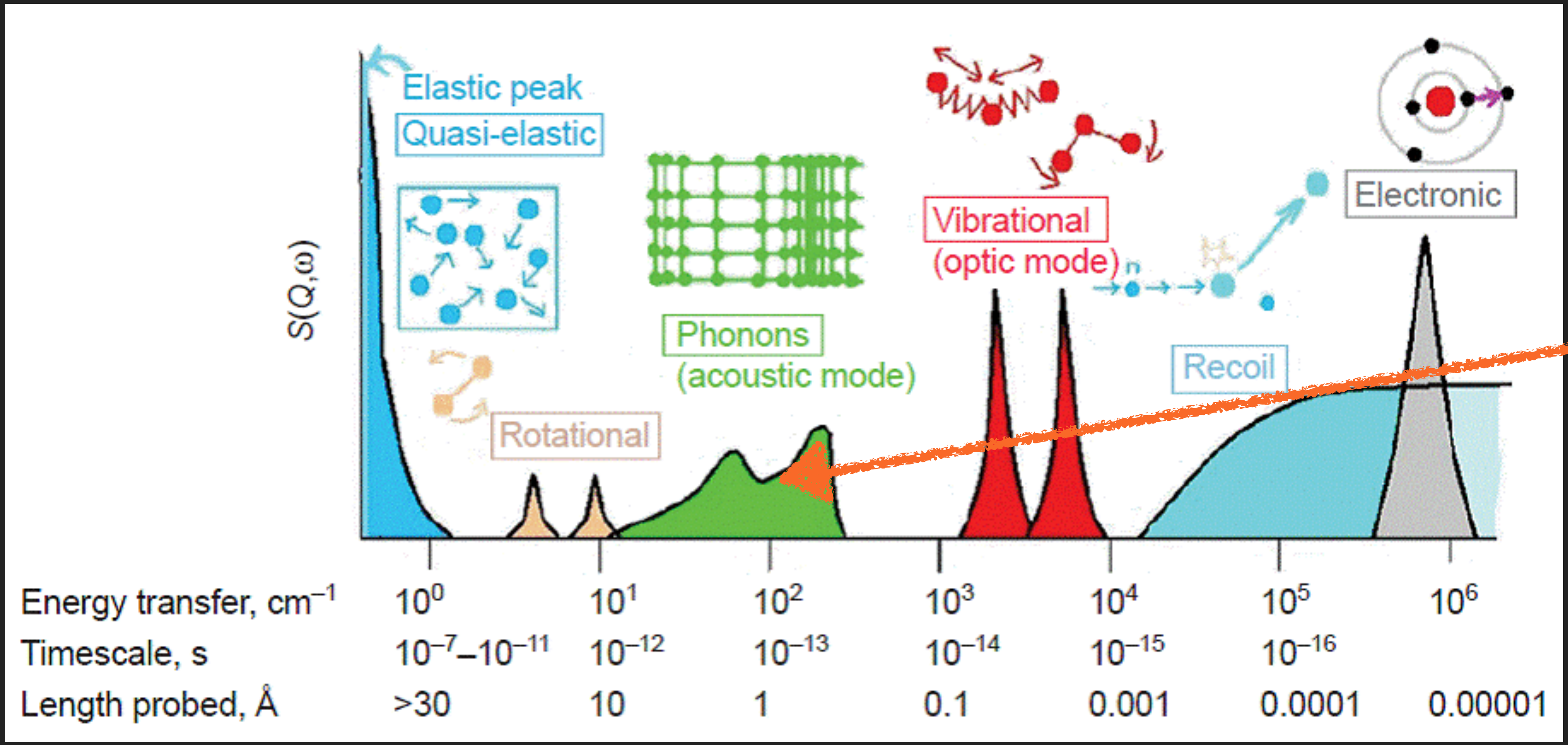
(PROF??) KEITH T. BUTLER

ANALYSING AND UNDERSTANDING INELASTIC NEUTRON SCATTERING WITH DEEP LEARNING

INELASTIC NEUTRON SCATTERING

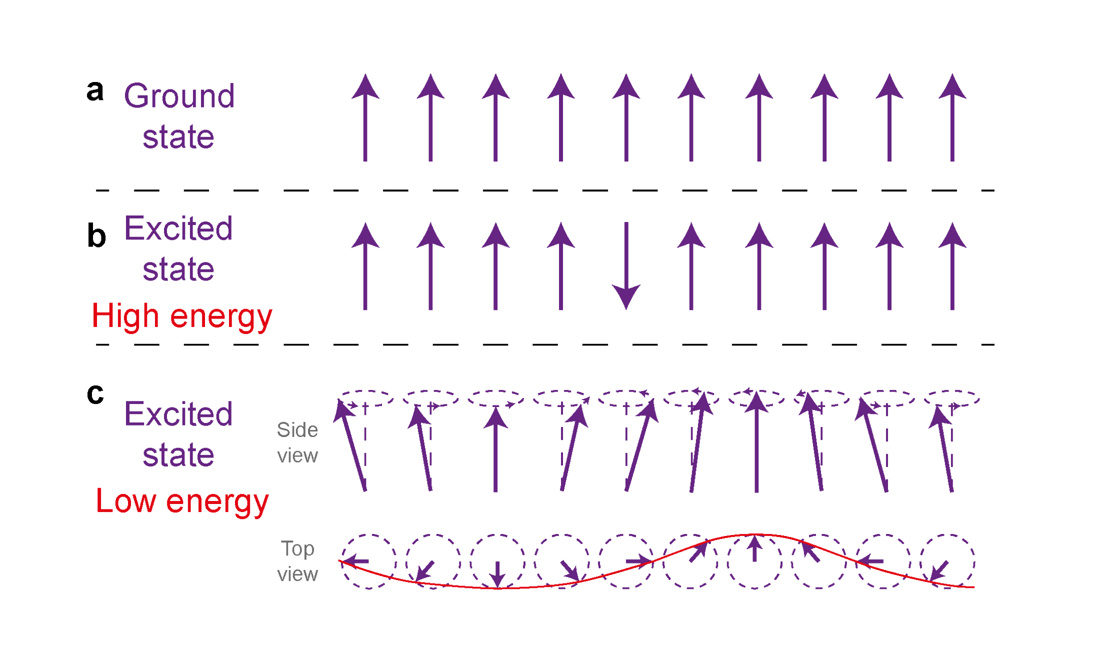
- Inelastic energy transfer can occur due to many processes
- Inelastic events give spectra

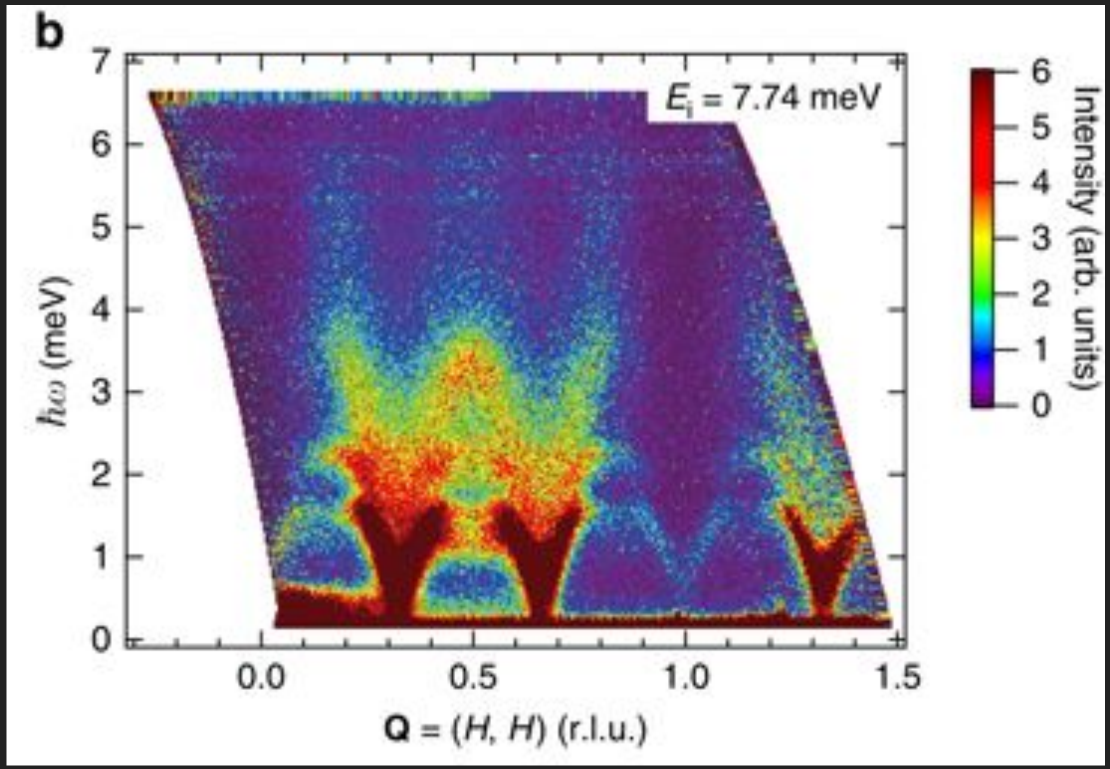


And magnons

MAGNONS

- Magnons are low energy excited states of electrons
- Spin on one electron is perturbed and propagates through the lattice resulting in a wave of reorganisation
- Dependent on the magnetic structure of a material

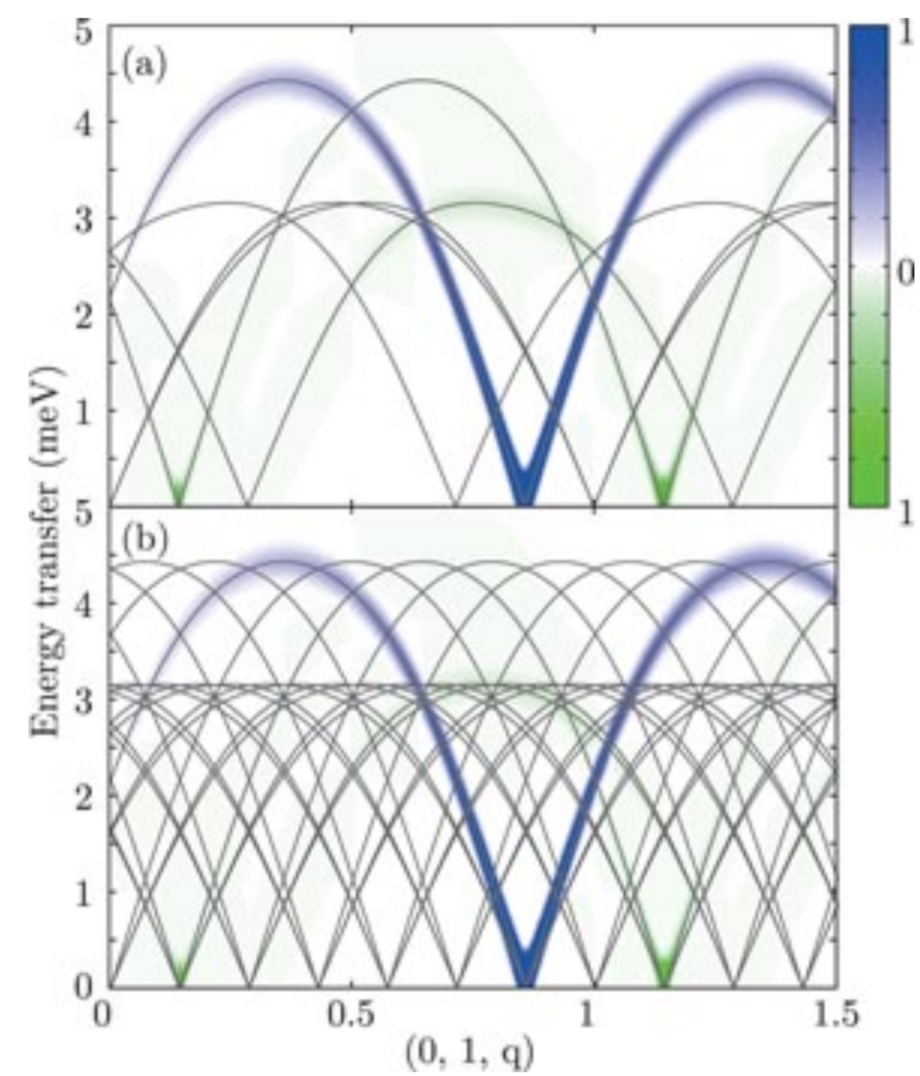




Nature Communications **volume 8**, Article number: 235 (2017)

SOLVING LINEAR SPIN WAVE THEORY: SPIN-W

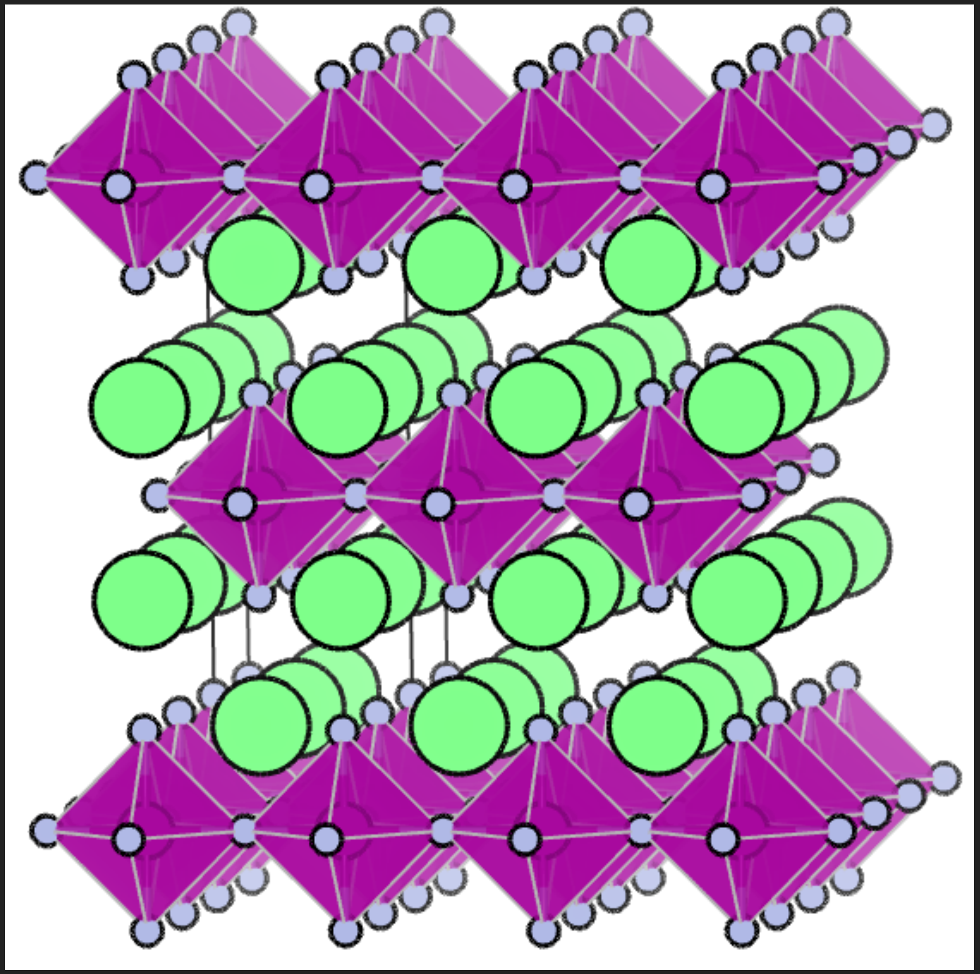
- Numerical solver for the linear spin wave Hamiltonian
- **Input** : Magnetic moments, lattice, model of interactions
- **Output**: Simulated spectrum - can numerically fit to experiment



Journal of Physics: Condensed Matter, Volume 27, Number 16

RB2MNF4

- 2D Antiferromagnet
- Interactions in planes of MnF
- Mostly described by linear spin wave theory

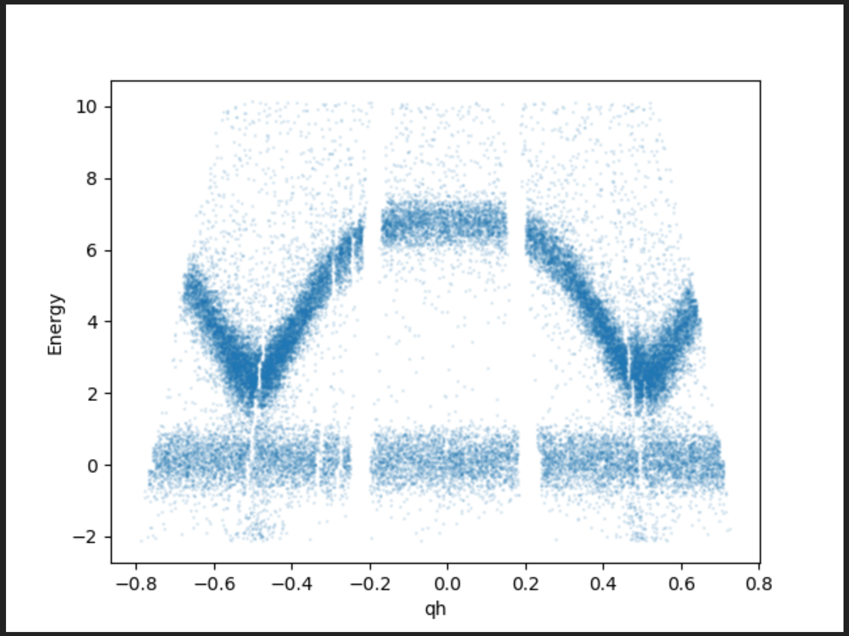


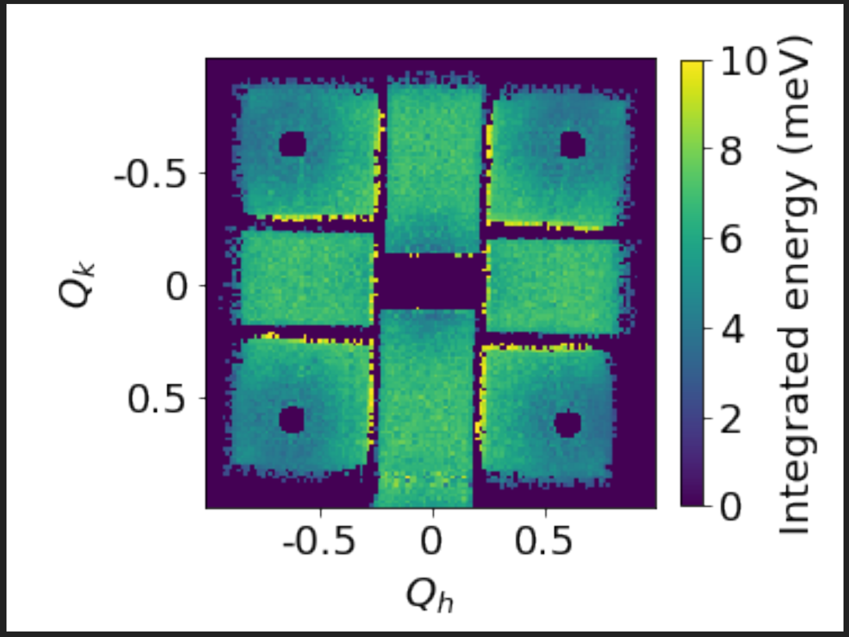
Two-magnon excitations observed by neutron scattering in the two-dimensional spin-$\frac{5}{2}$ Heisenberg antiferromagnet $\mathrm{Rb_2\,Mn\,F_4}$

T. Huberman, R. Coldea, R. A. Cowley, D. A. Tennant, R. L. Leheny, R. J. Christianson, and C. D. Frost
Phys. Rev. B **72**, 014413 – Published 6 July 2005

RB2MNF4 THE DATA

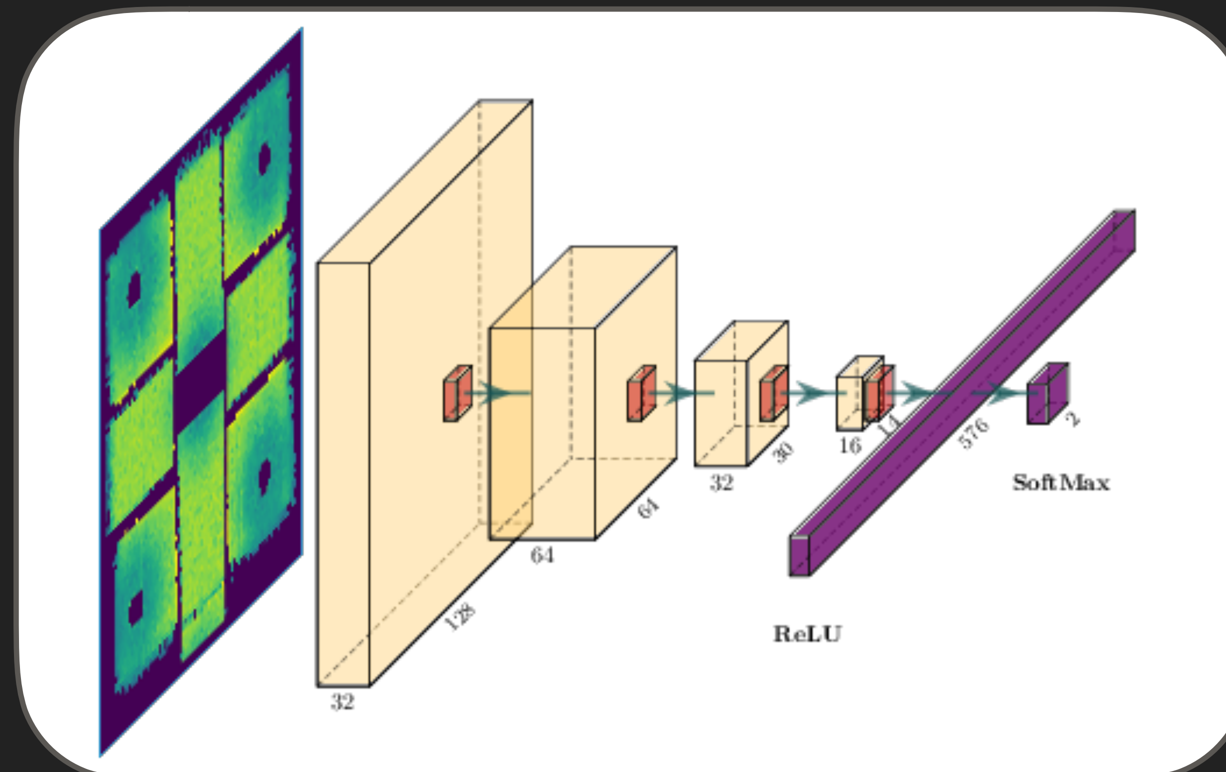
- Clean data-set
- Single magnon dispersion band
- Remove Bragg peaks and integrate the signal intensity across the energy range
- 2D map in Qh/Qk
- Can we train a model to estimate the exchange constants?





RB2MNF4 RESULTS

- Simple neural network with 4 convolutional layers - extract features
- Function approximation from two layer MLP



Literature values:

- $J_1 = 0.657 \pm 0.002$
- $J_2 = 0.006 \pm 0.003$

or:

- $J_1 = 0.673 \pm 0.028$
- $J_2 = 0.012 \pm 0.002$

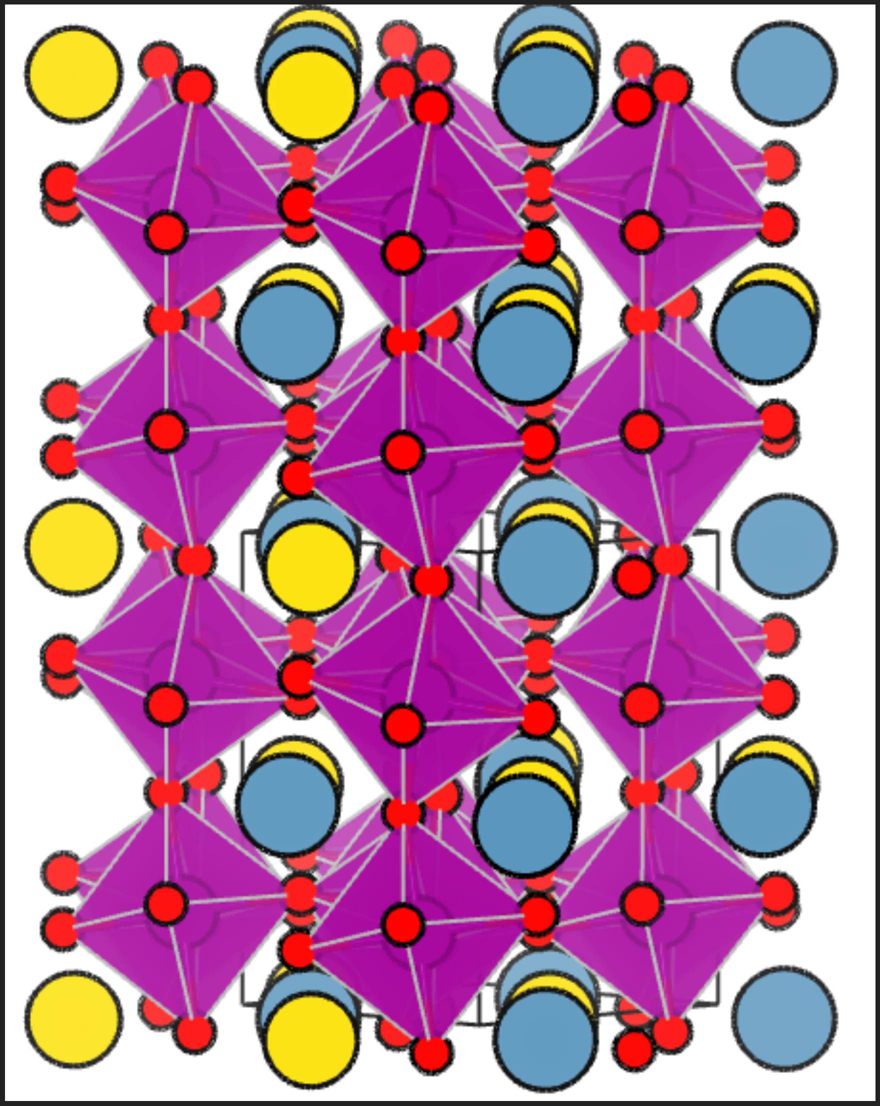
$$J_1 = 0.676$$
$$J_2 = 0.014$$

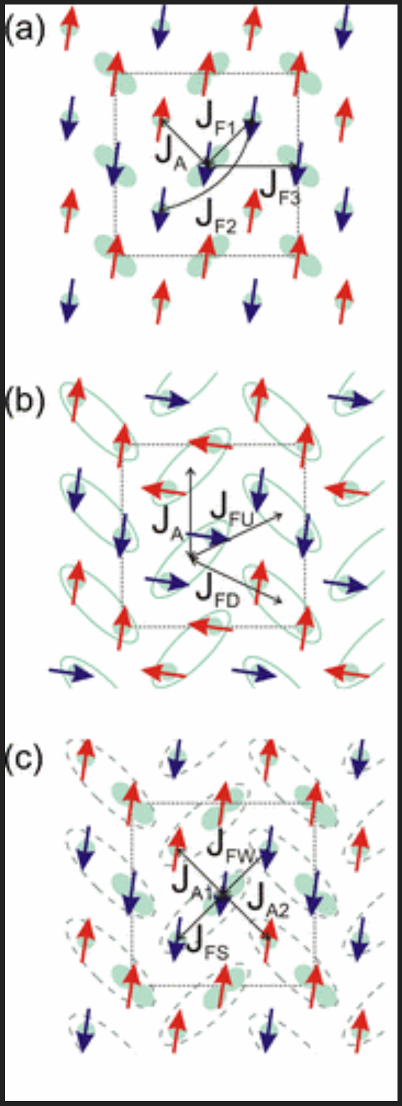
PCSMO THE SYSTEM

- Double perovskite
- Mixed A-site
- Several possible models for the magnetism
- Goodenough model
- Zener polaron
- Dimer model

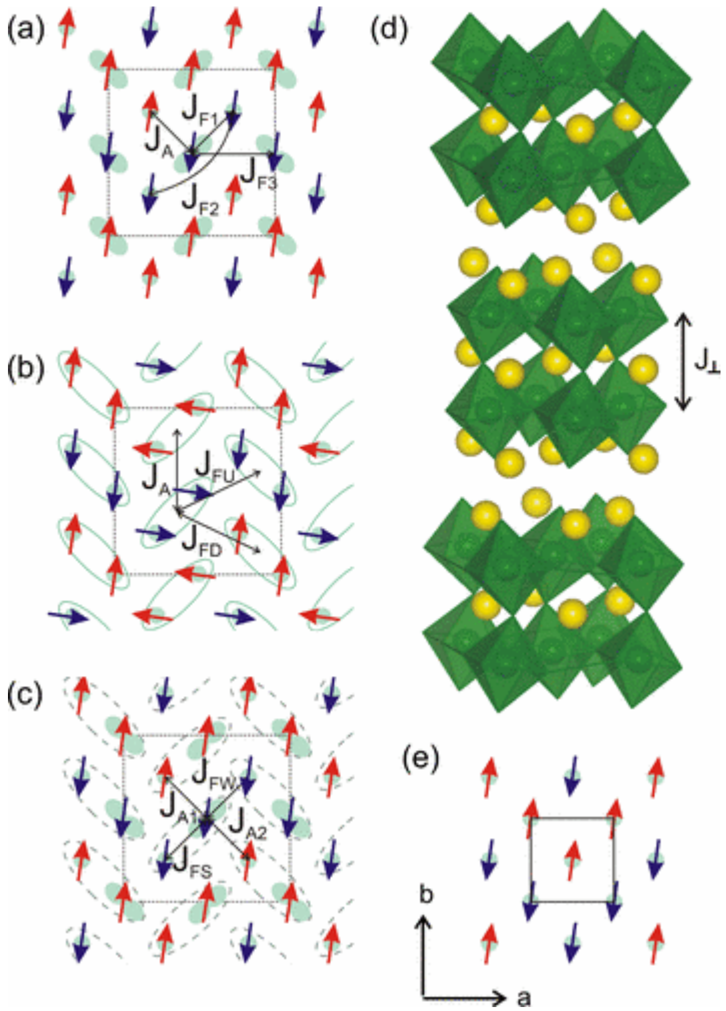
Ground State in a Half-Doped Manganite Distinguished by Neutron Spectroscopy

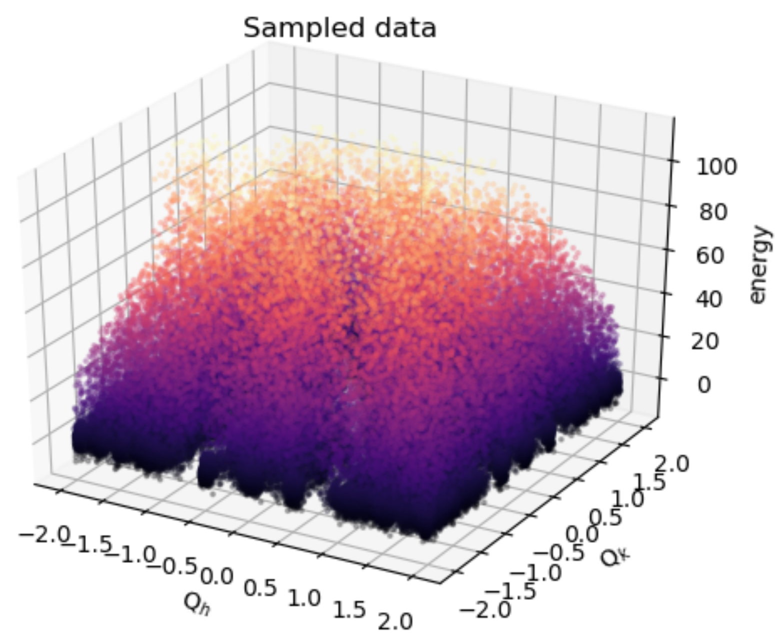
G. E. Johnstone, T. G. Perring, O. Sikora, D. Prabhakaran, and A. T. Boothroyd
Phys. Rev. Lett. **109**, 237202 – Published 3 December 2012



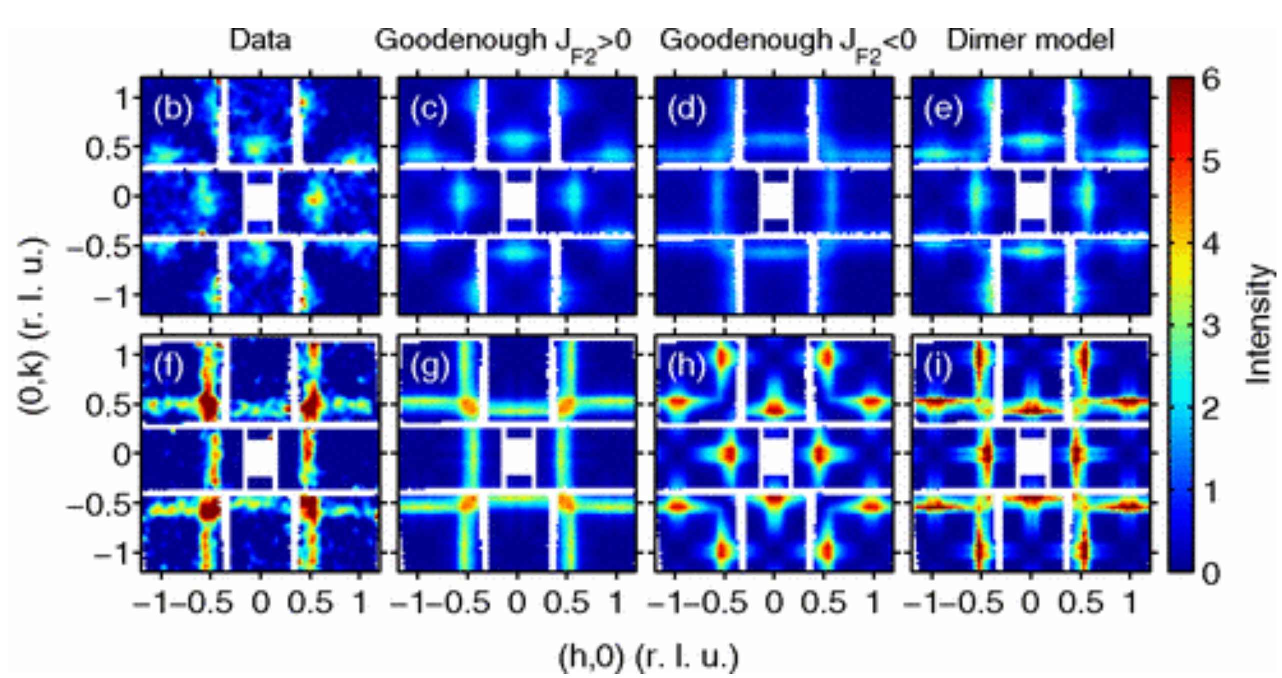


CAN WE FIND THE RIGHT DATA TO DISCRIMINATE



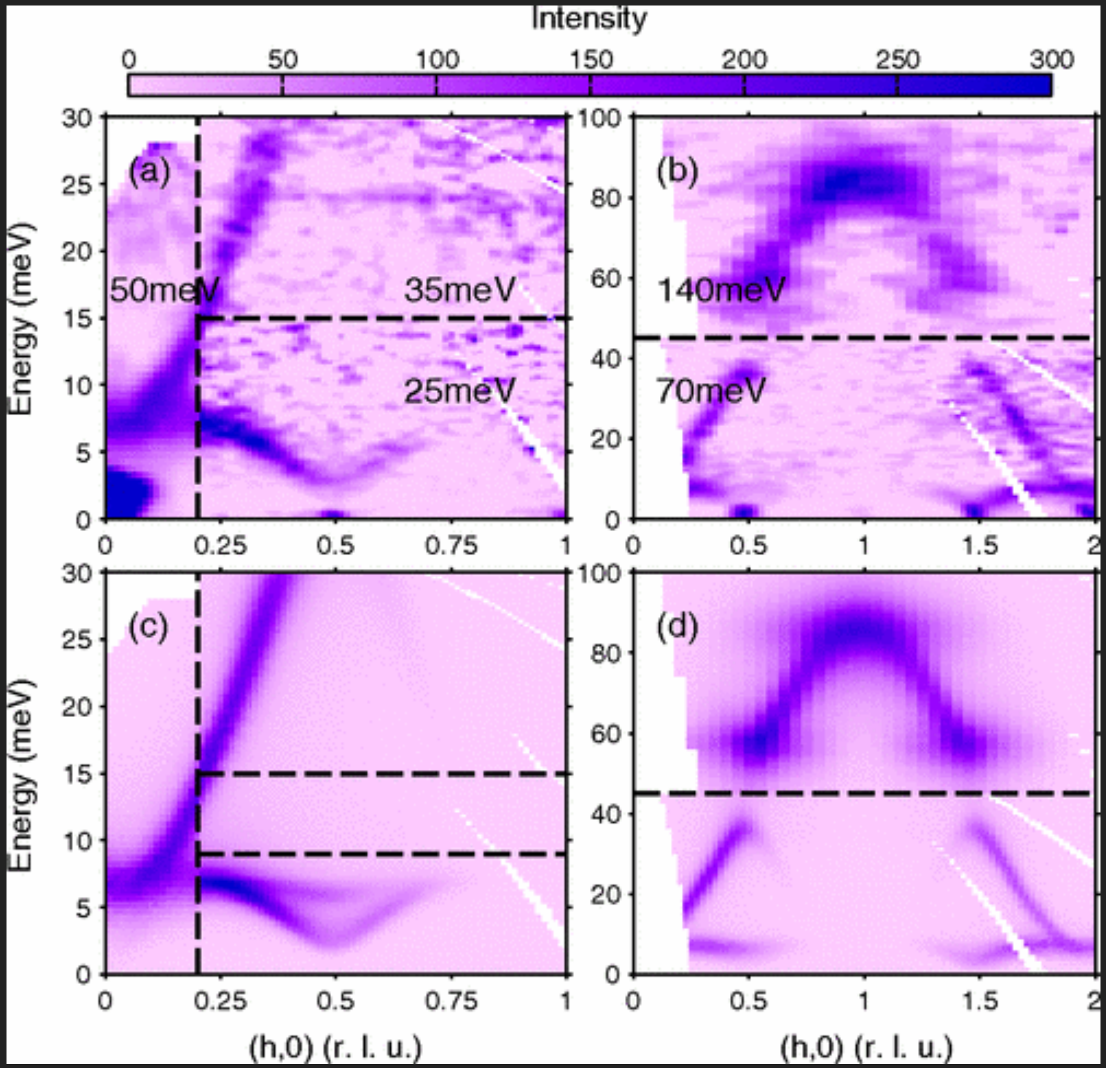


Finding the right signal can be a needle in a haystack



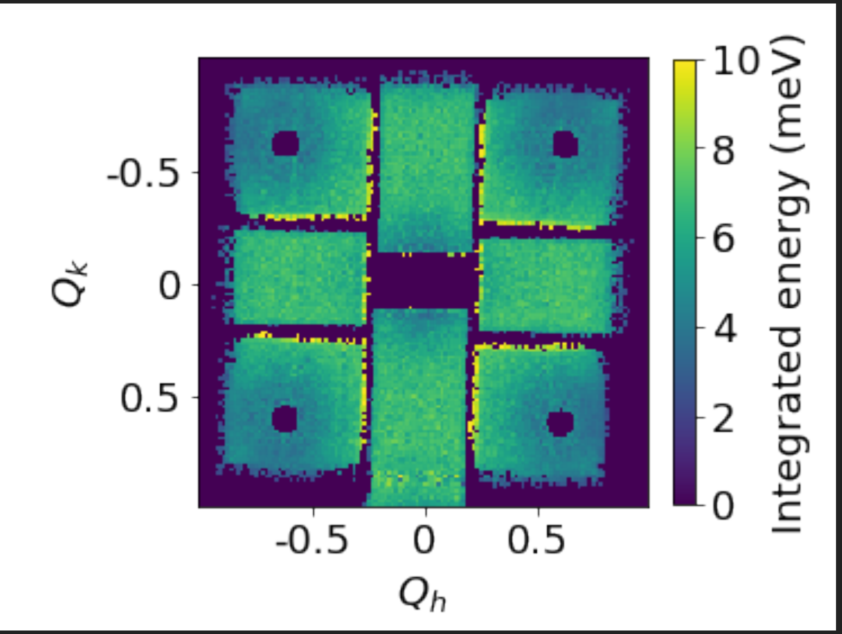
PCSMO THE DATA

- Significantly messier dataset
- Noisy experimental data
- Multiple bands
- Presence of phonons



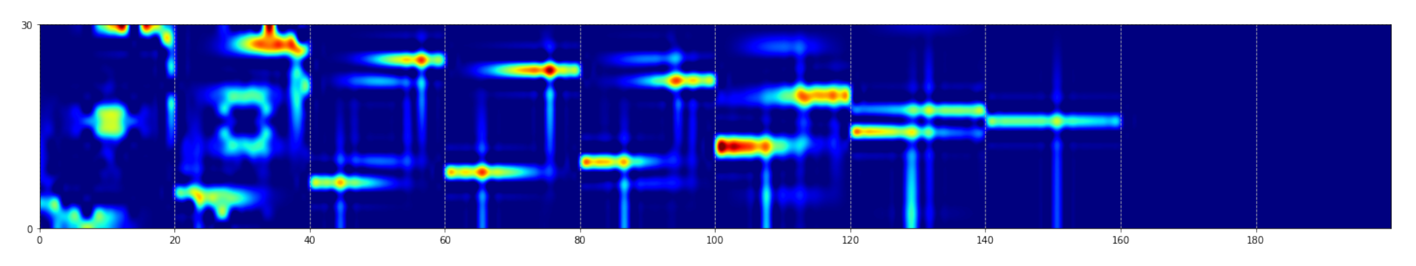
PCSMO THE DATA PART II: MULTI-BANDS AND HOW TO DEAL WITH THEM

- In Rb2MnF4 we could integrate across the energy spectrum

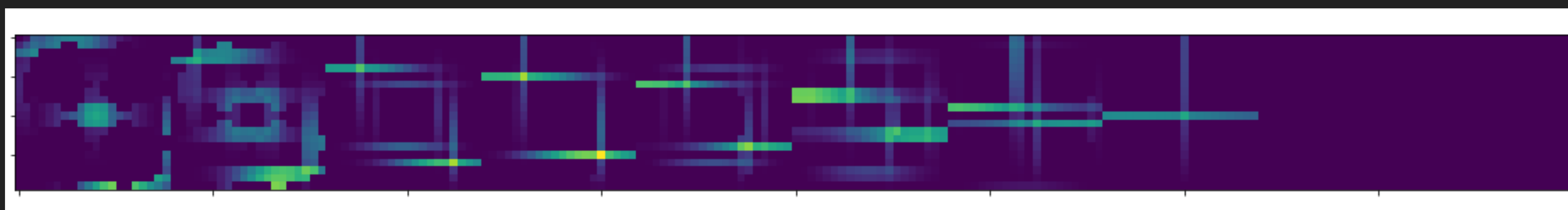


- In PCSMO this would lead to loss of information

- Develop an image with interactions across energy slices



PCSMO RESULTS: PHASE DISCRIMINATION (SIMULATED DATA)

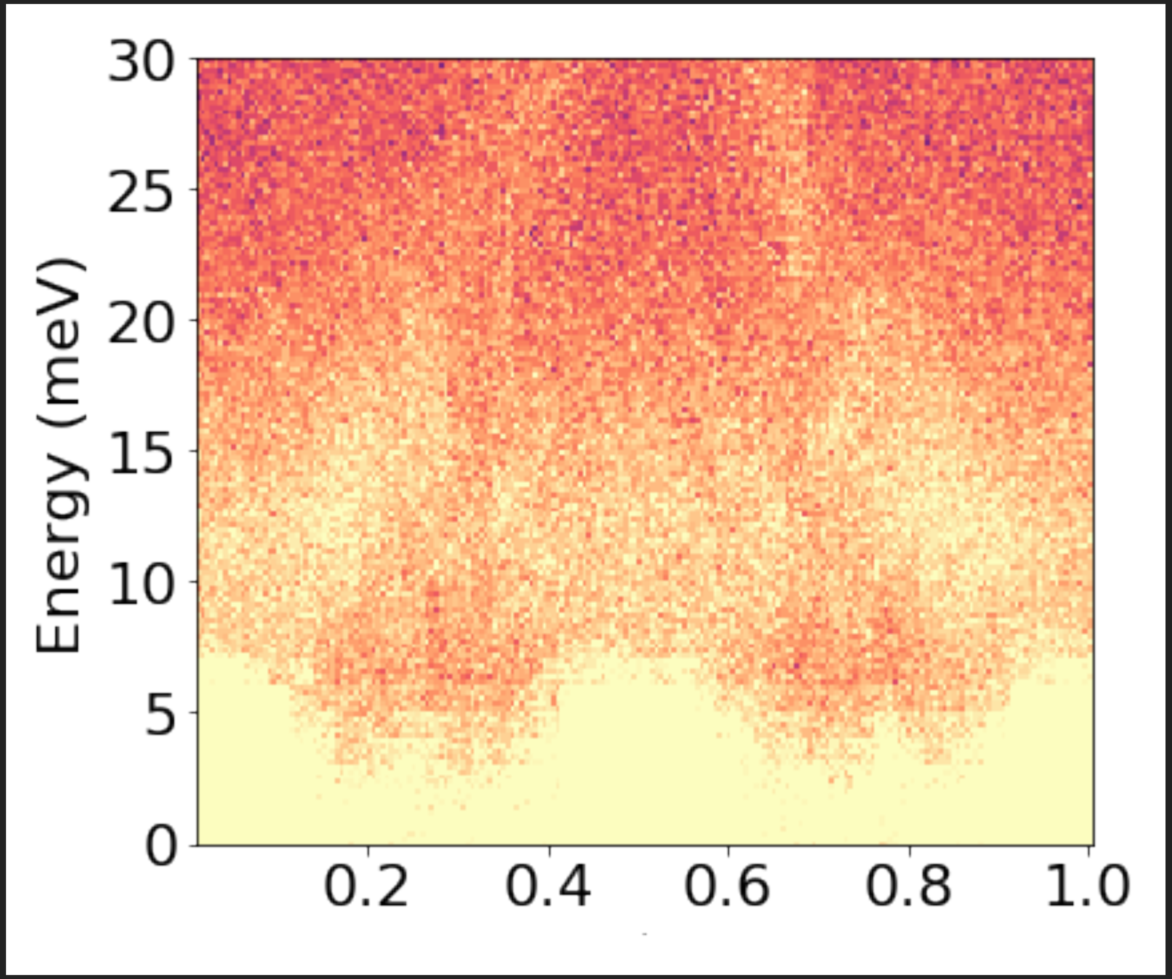


```
[conv_outputs, predictions] = get_output([test_i
conv_outputs = conv_outputs[0, :, :, :]
maxval = np.argmax(np.array(predictions))
```

```
Prediction Goodenough
```

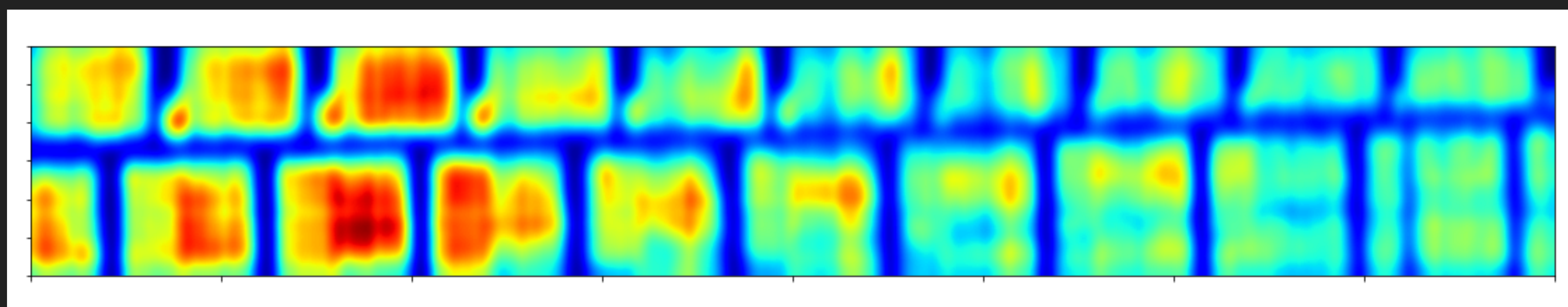
PCSMO THE DATA PART III : "NOISE"

- There is a large contribution from the phonon spectrum
- This can obfuscate the magnon spectrum
- Would like to remove this if possible



PCMSO RESULTS II: EXPERIMENTAL DATA

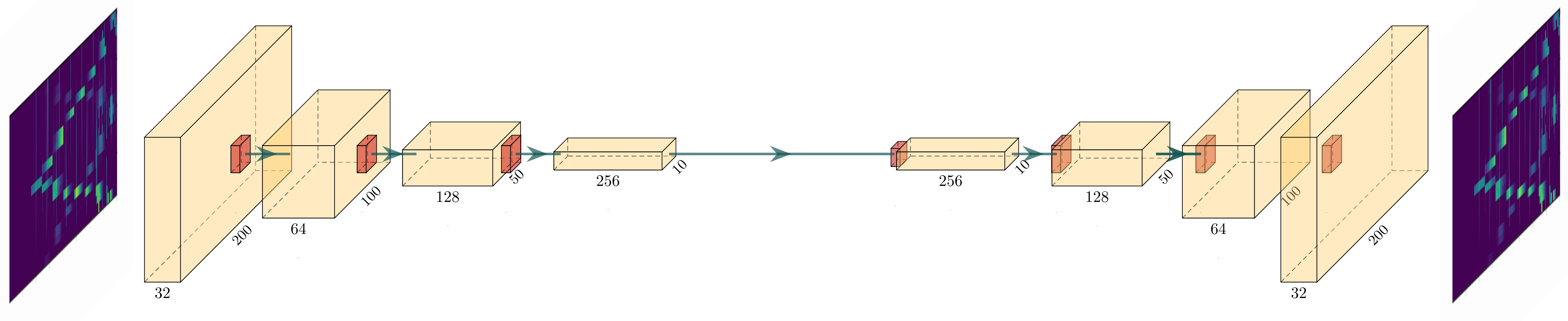
- Failure - noise :(



```
ylist = np.linspace(0, dim[0]*2, c
X, Y = np.meshgrid(xlist, ylist)
## Add Gaussian smoothening to con
sigma = 0.2 # this depends on how
camg = gaussian_filter(cam, sigma)
```

```
Prediction Dimer
[[8.2898813e-01 4.3244651e-08]]
```

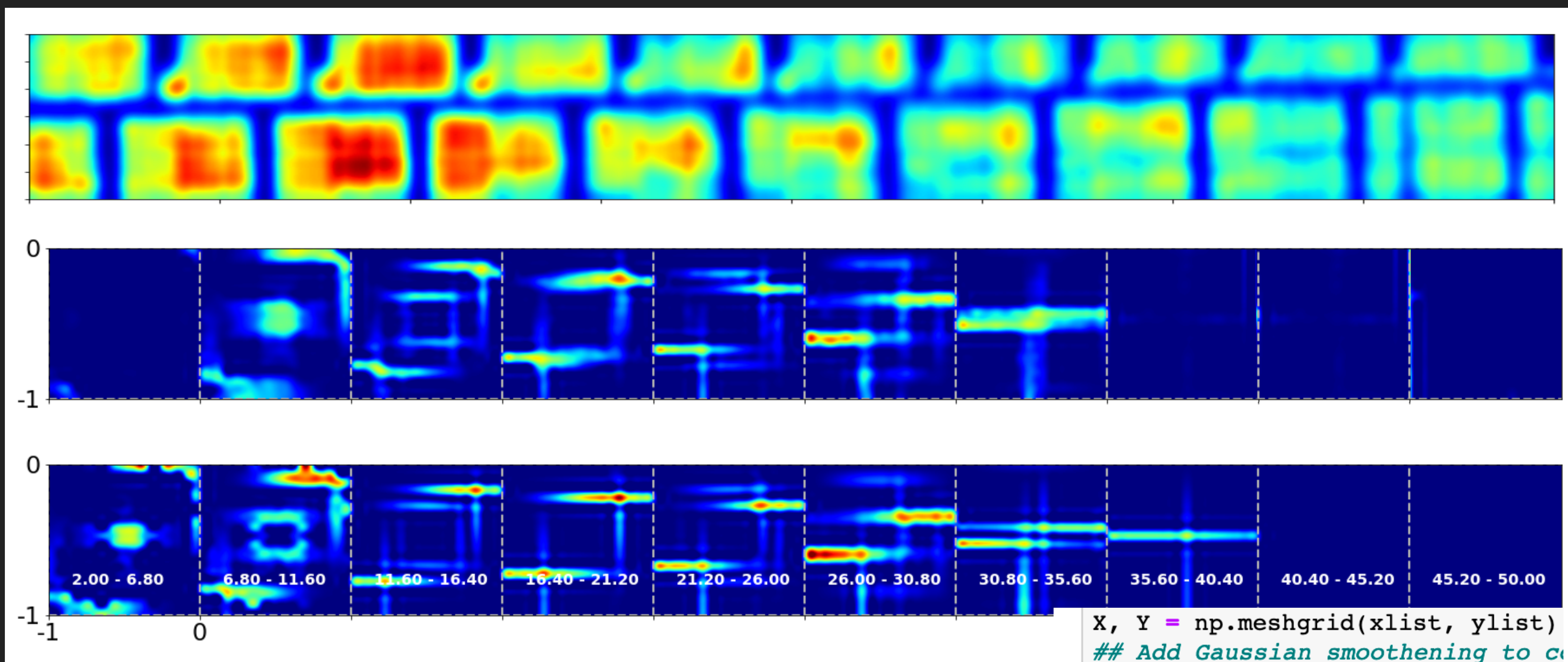
PCSMO: REMOVING THE NOISE (AUTOENCODERS)



- Can we remove the experimental 'noise'
- Noise = instrument noise + other signals
- We can try to use a denoising auto encoder

PCSMO RESULTS III: AUTOENCODER + DISCRIMINATION

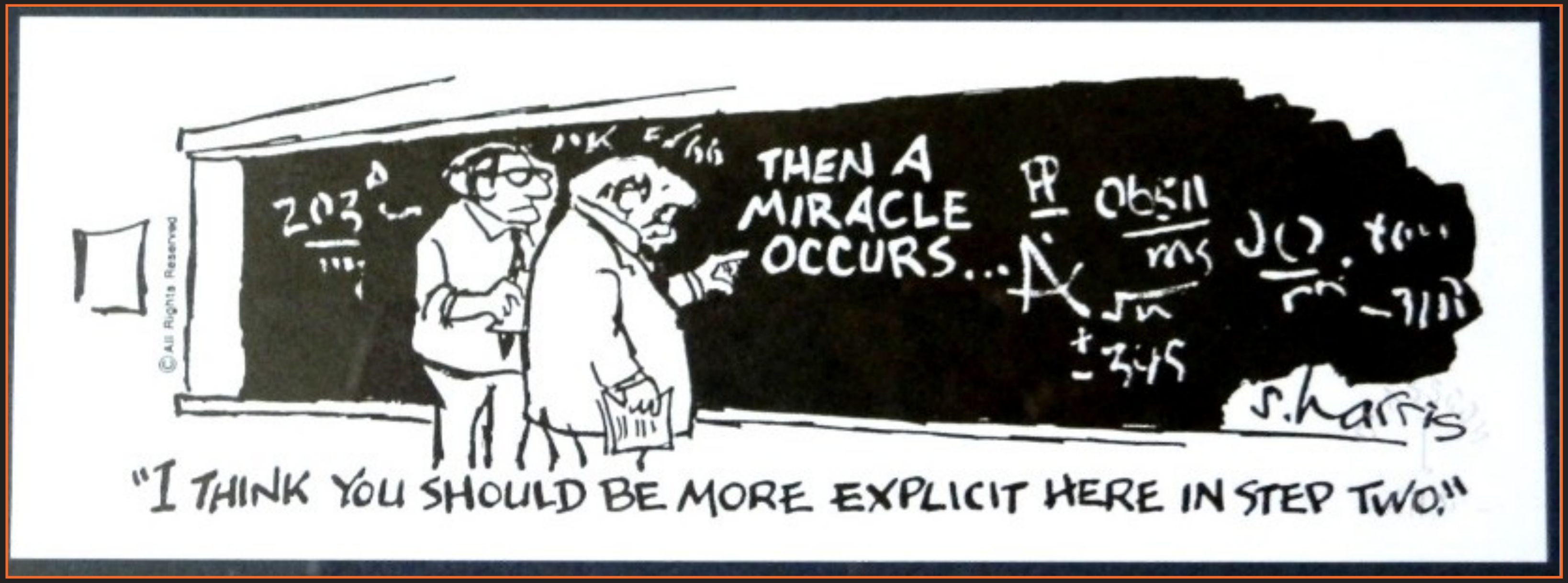
- (Qualified) Success :)




```
X, Y = np.meshgrid(xlist, ylist)
## Add Gaussian smoothening to co
sigma = 0.2 # this depends on how
camg = gaussian_filter(cam, sigma
```

```
Prediction Goodenough
[[0.00203549 0.90476966]]
```

MAKING MODELS INTERPRETABLE



- Classical models are often easy to interpret

- Deep models, learned representations can be more opaque

MAKING MODELS INTERPRETABLE

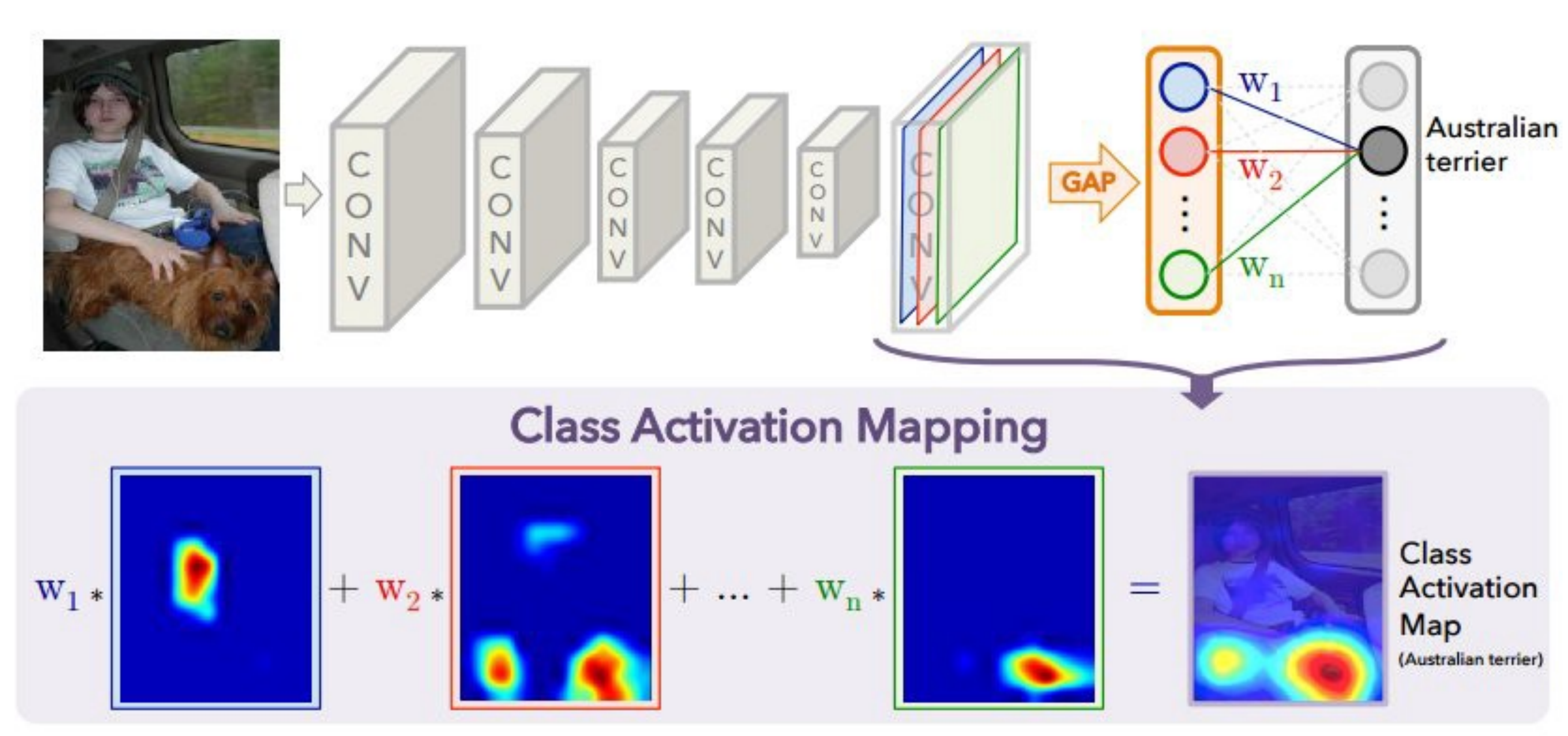
Model performance	Interpretability use
Sub-human	Debug and improve
Human	Increase confidence
Super-human	Learn from successs

CLASS ACTIVATION MAPS

- Show which regions of an input are responsible for classification

arXiv:1512.04150v1

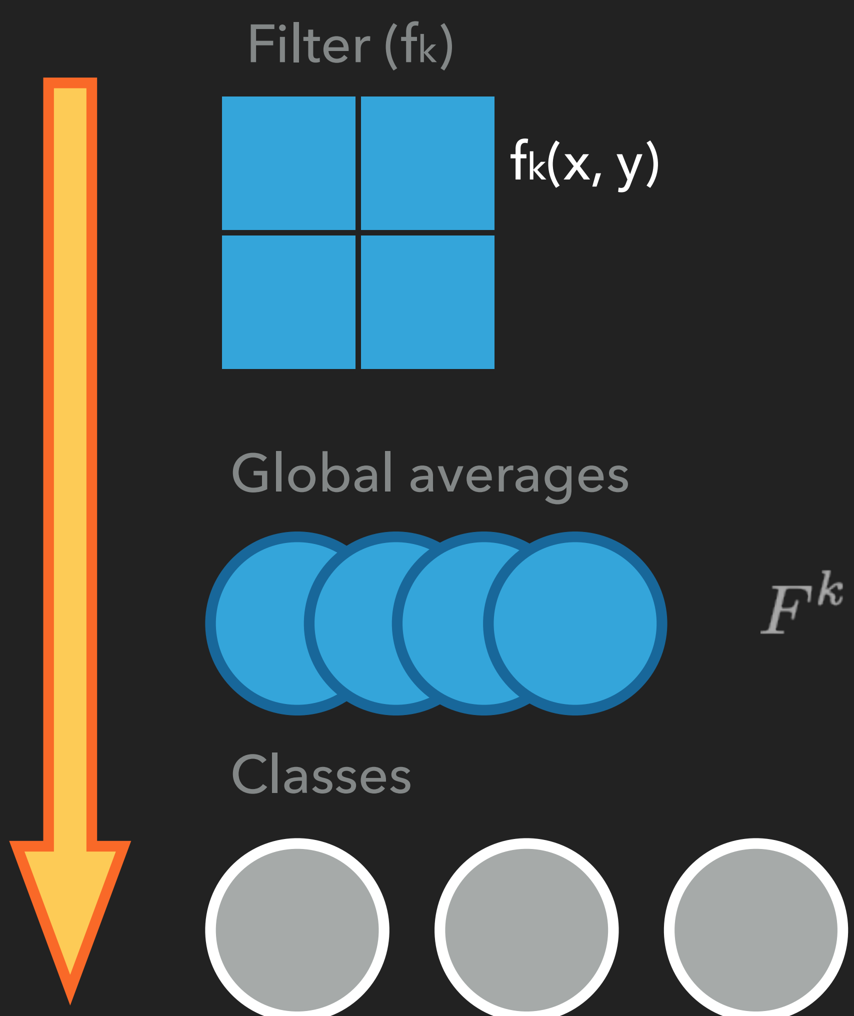
CLASS ACTIVATION MAPS NETWORK ARCHITECTURE



- Global average pooling
- Apply to final convolutional layer

arXiv:1512.04150v1

CAM HOW IT WORKS



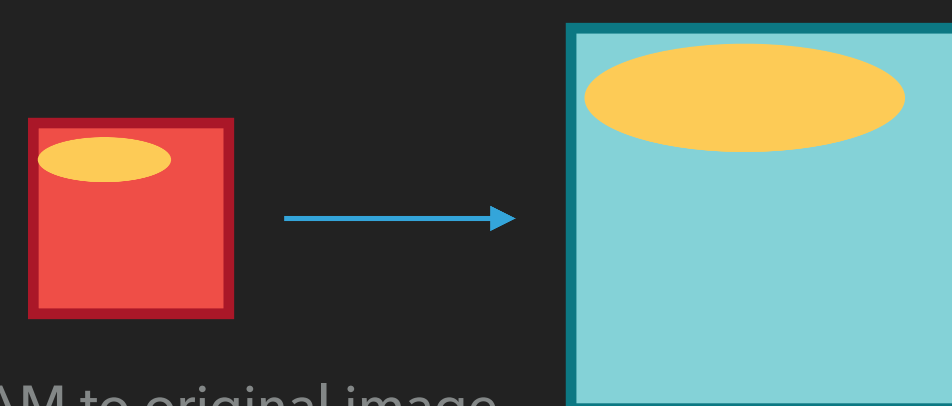
$$F^k = \sum_{x,y} f_k(x, y)$$

$$S_c = \sum_k w_k^c F^k$$

$$S_c = \sum_k \sum_{x,y} w_k^c f_k(x, y)$$

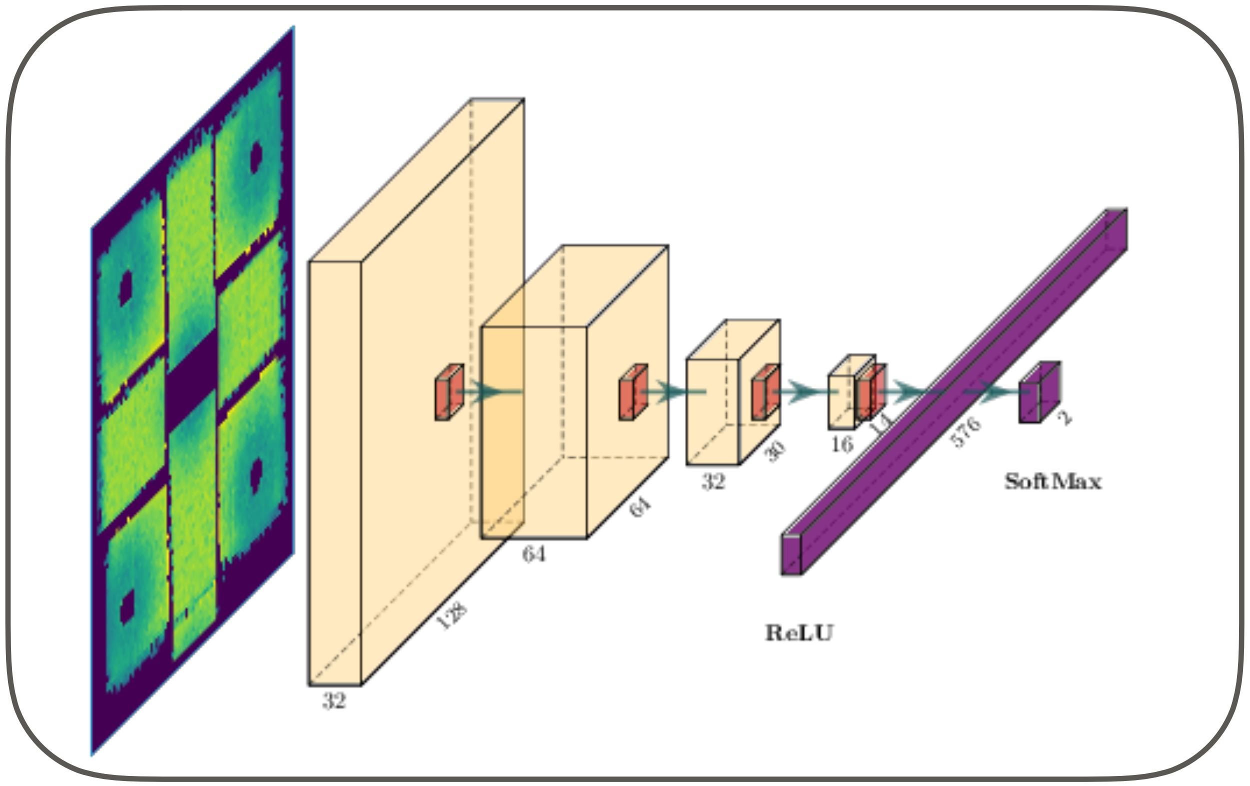
$$M_c(x, y) = \sum_k w_k^c f_k(x, y)$$

Directly indicates the importance of a location (x, y) to the class activation S_c.

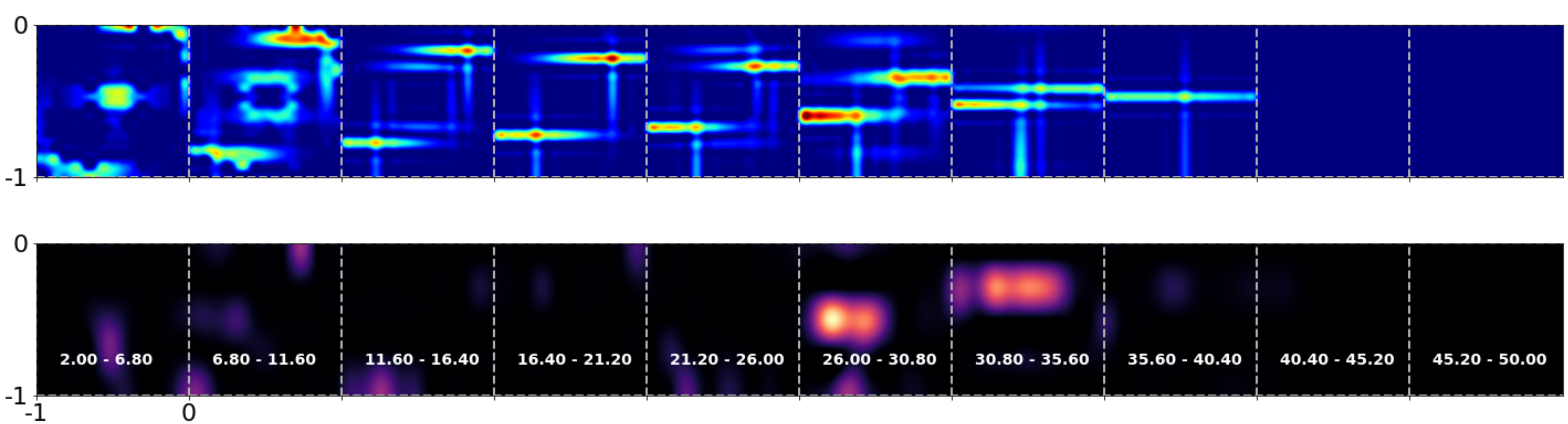


Upsample CAM to original image size

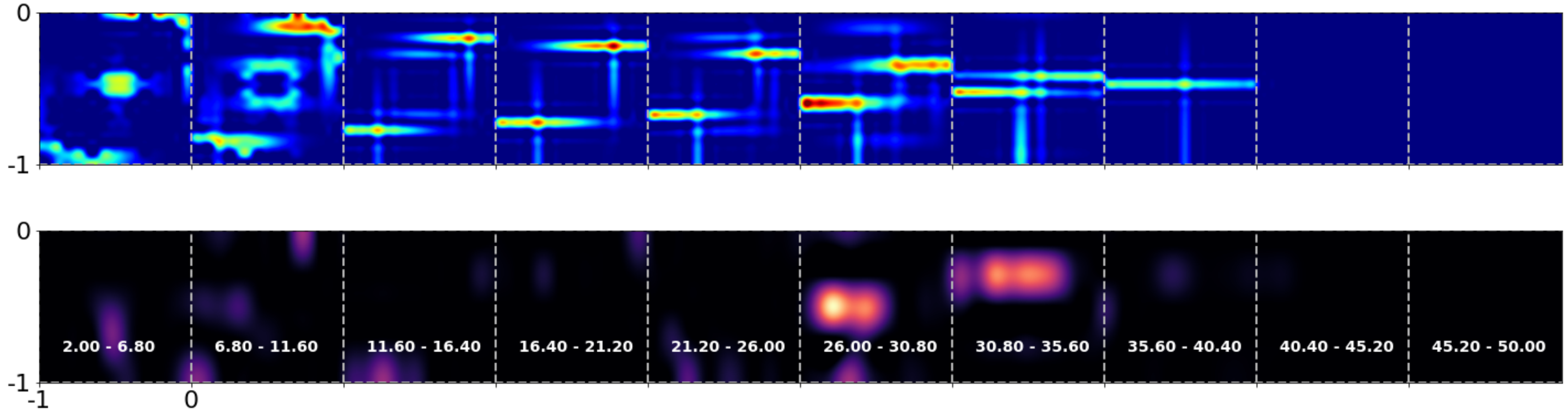
INTERPRETABLE MODELS FOR NEUTRON SCATTERING

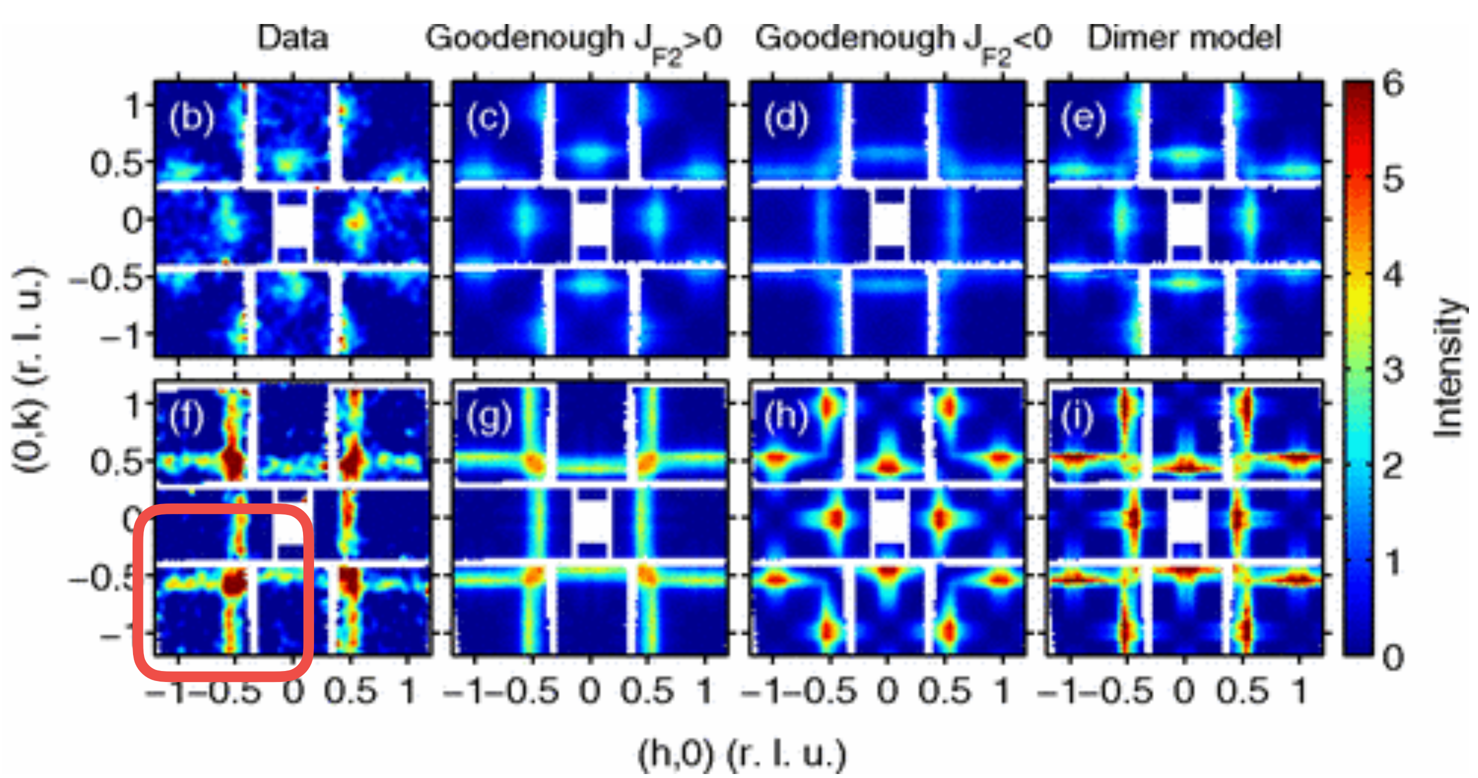


Build a model discrimination network - ask it WHY it makes the choice.



INTERPRETABLE MODELS FOR NEUTRON SCATTERING





The network identifies the same regions of E/Q space as a trained physicist.

Could, in future, guide experiments of the same type.

SUMMARY

- Inelastic neutron scattering requires complex data analysis to extract useful information
- Combining physics simulations with deep neural networks can help in interpreting experimental spectra
- Understanding how neural networks arrive at answers is generally a good idea!
- Understanding network results can provide guidance on how to sample experimental space

ACKNOWLEDGMENTS

- SciML
  - Rebecca, Tony, Jeyan, Sam, Patrick
- ISIS
  - Duc, Toby

THANK YOU

"When we apply for funding it's AI, when we hire it's machine learning and when we do the work it's logistic regression"

Anon - Twitter wisdom

@keeeto2000
@ml_sci

keeeto.github.io

www.scd.stfc.ac.uk/Pages/Scientific-Machine-Learning.aspx