Machine Learning Phases of Strongly-Correlated Fermions

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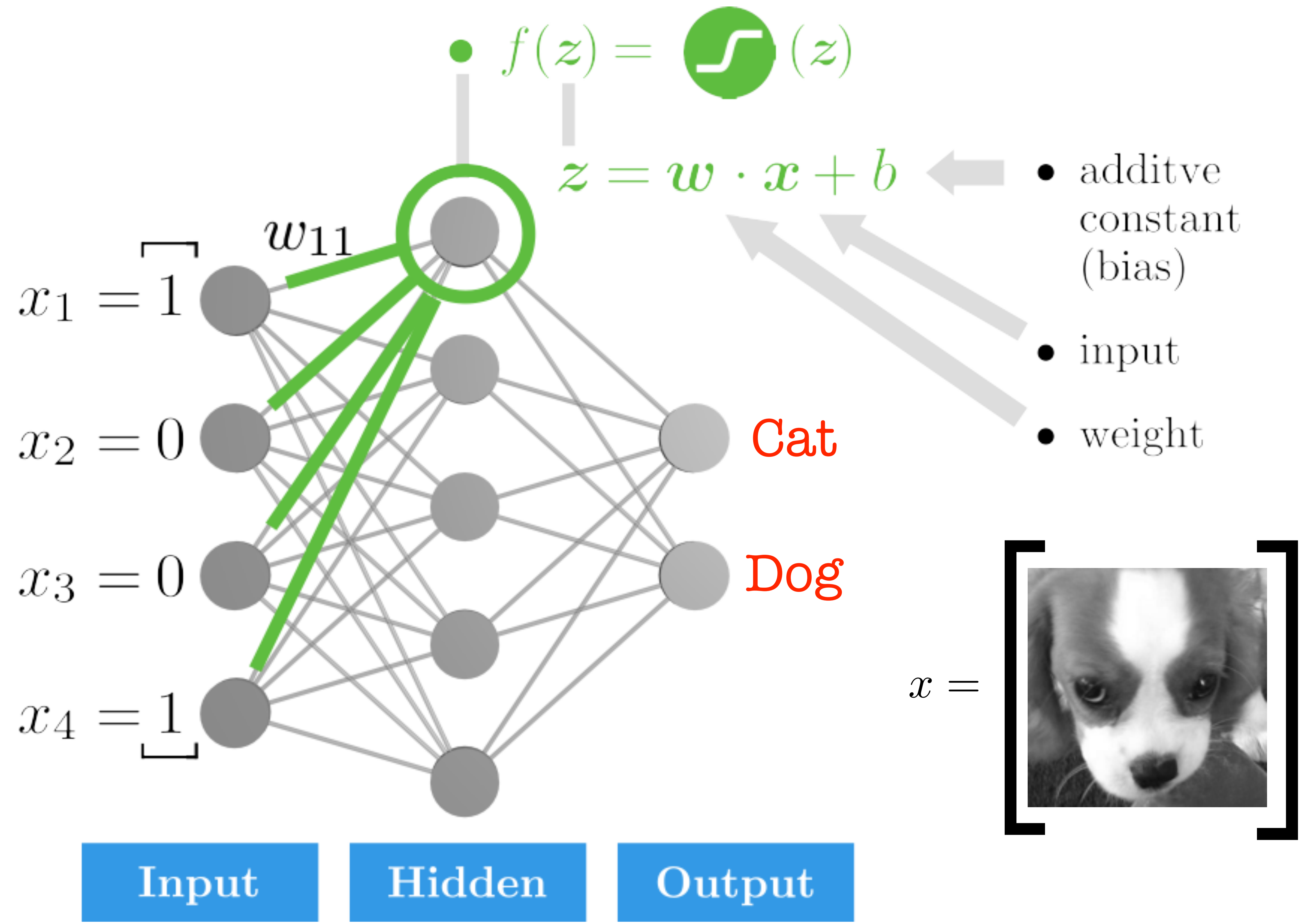
Machine Learning and Many-Body Physics

KITS Beijing, July 3, 2017

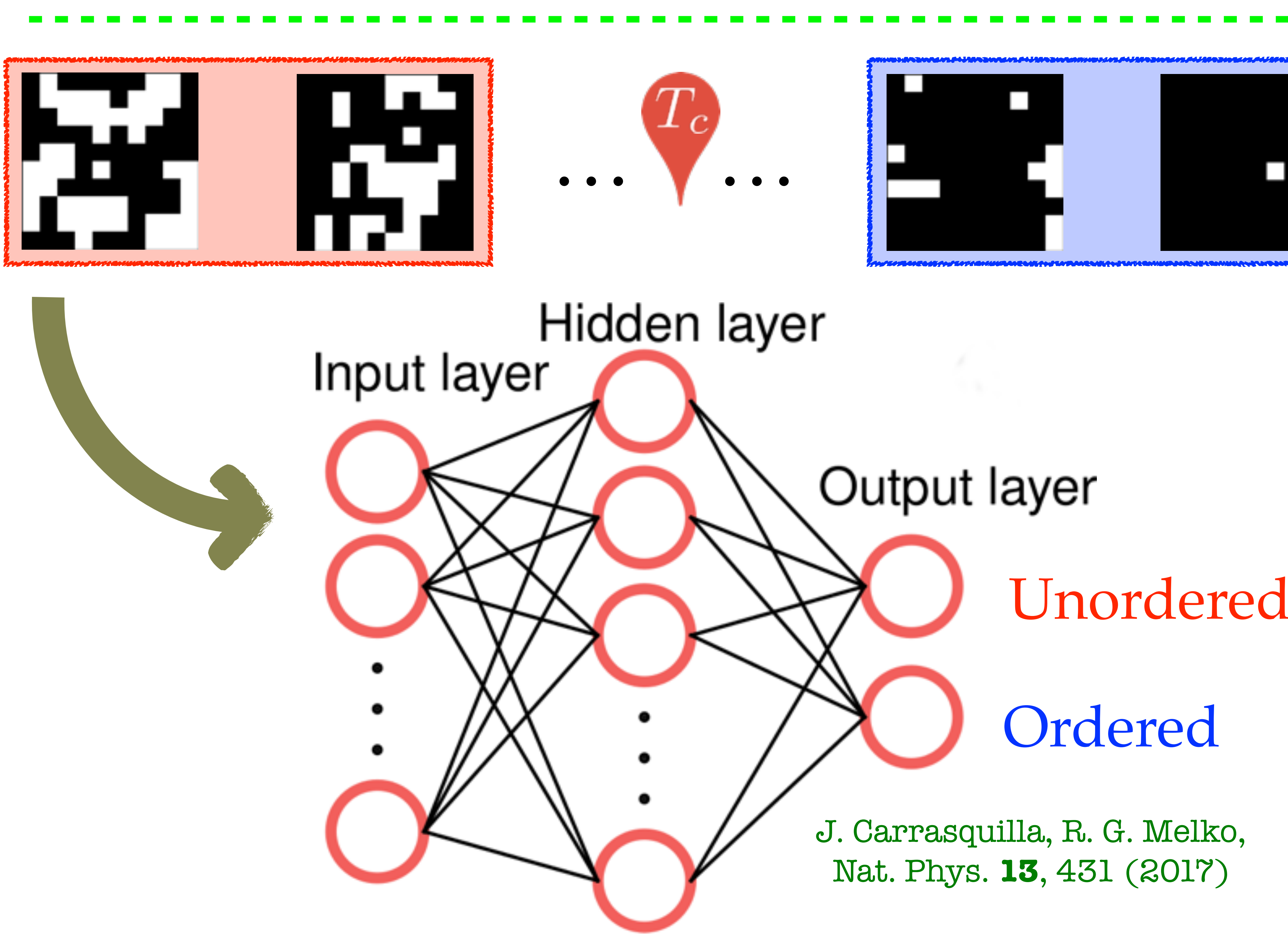
K. Ch'ng, J. Carrasquilla, R. G. Melko, EK, arxiv 1609.02552

Artificial Neural Networks



ML and Many-Body Physics

Ising configurations at decreasing temperatures

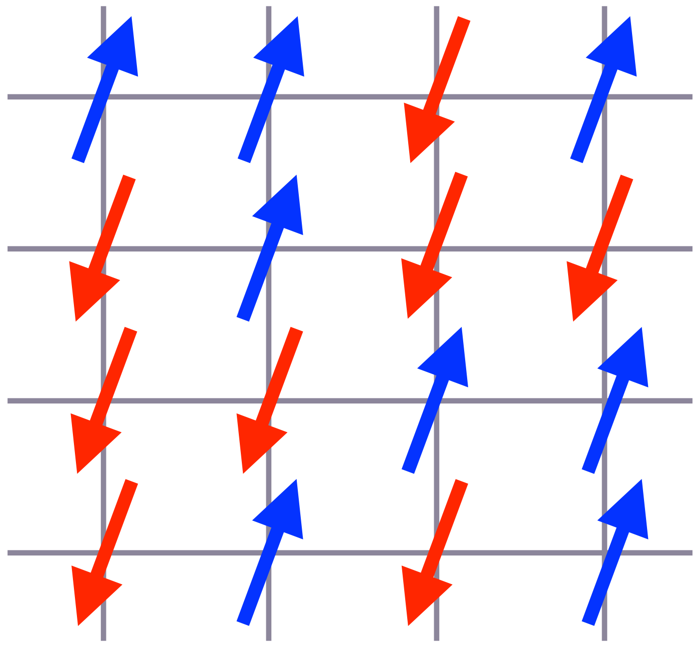


J. Carrasquilla, R. G. Melko,
Nat. Phys. **13**, 431 (2017)

2D Ising Model

$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \qquad (\sigma_i = \pm 1)$$

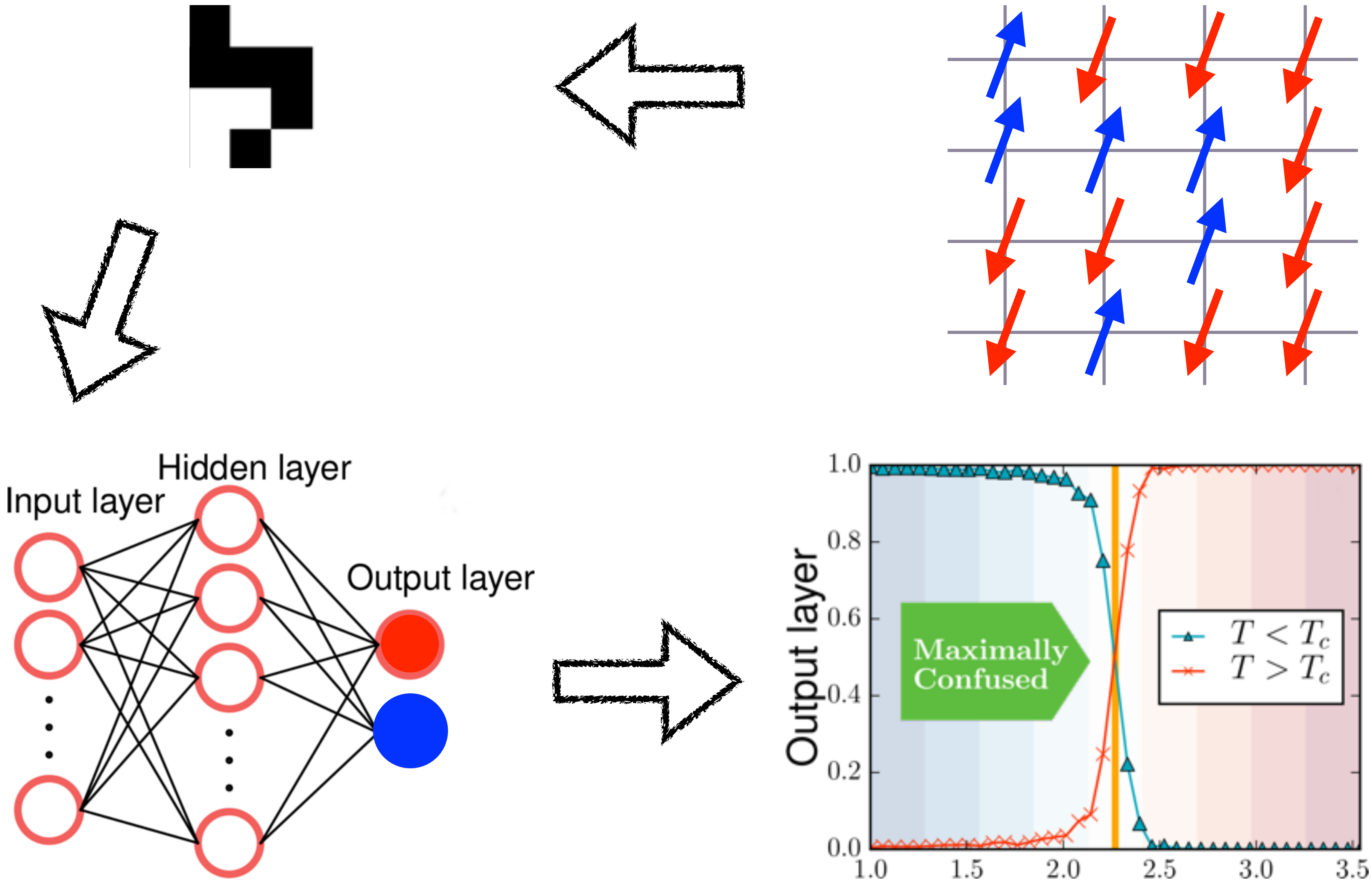
$$\langle O \rangle = \frac{1}{Z} \sum_{\{\sigma\}} O e^{-\beta H} \qquad (\beta = 1/T)$$



Take the sum stochastically using the Metropolis algorithm:

- Start with a random configuration
- propose a spin flip
- Accept the change if $e^{-\beta \Delta H} > r$ $\qquad 0 < r$ (random #) < 1
- Average the property of interest over configurations

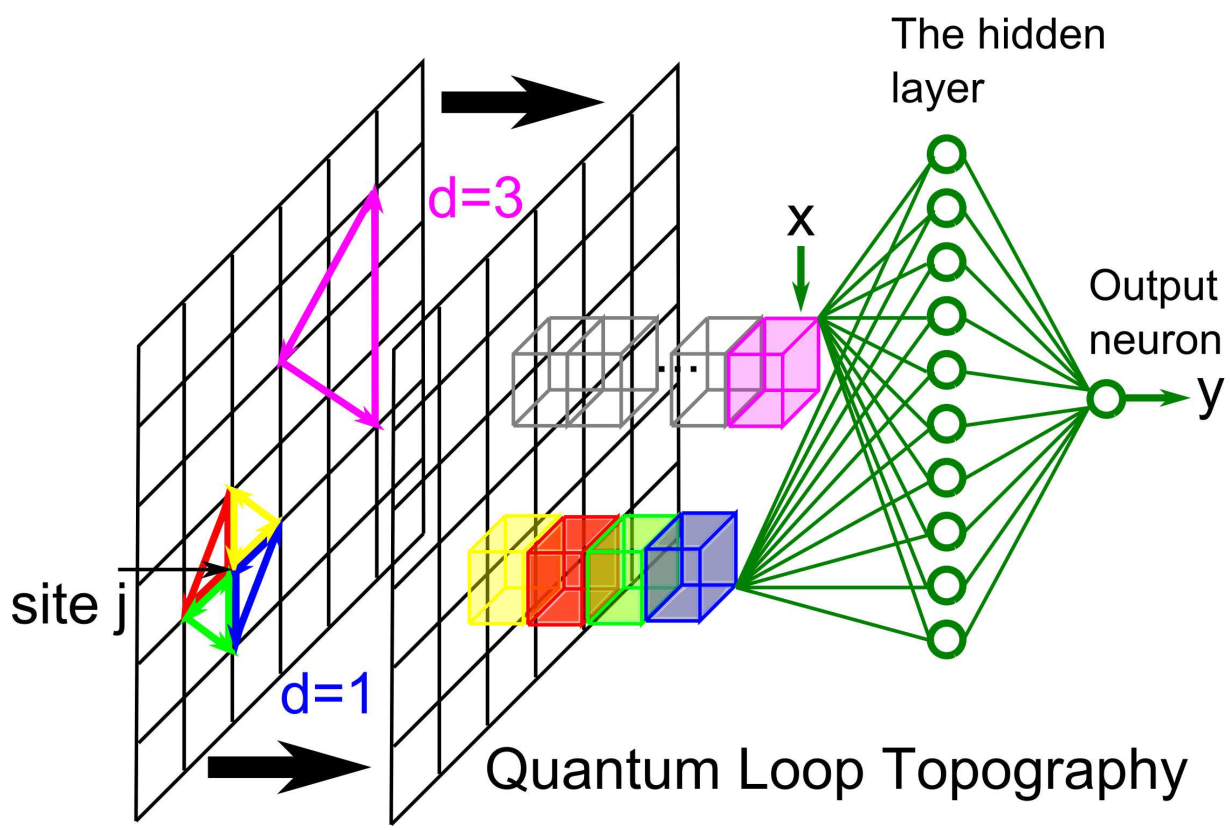
2D Ising Model

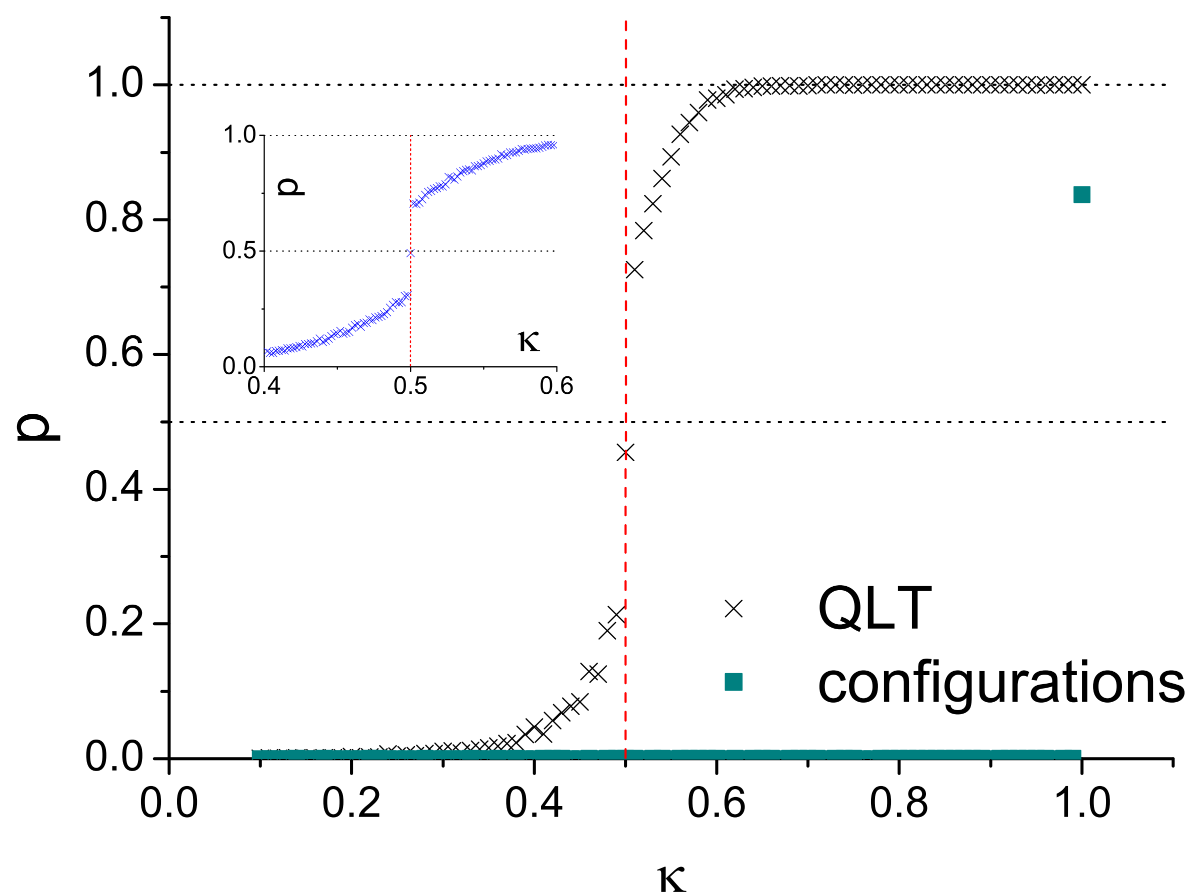


J. Carrasquilla, R. G. Melko, Nat. Phys. **13**, 431 (2017)

Finding Tc with 99% accuracy

Detecting Topological Order

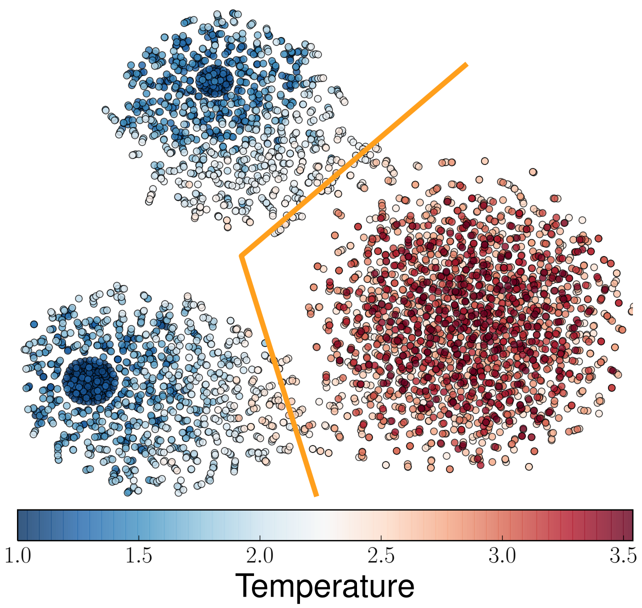




Y. Zhang, E. Kim, Phys. Rev. Lett. **118**, 216401 (2017)
Y. Zhang, R. G. Melko, E. Kim, arXiv:1705.01947

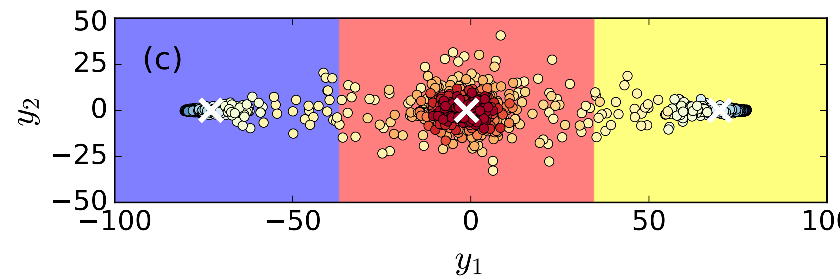
Unsupervised Learning

t_SNE



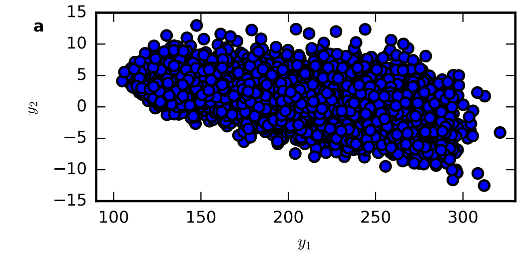
J. Carrasquilla and R. G. Melko,
Nature Physics **13**, 431-434 (2017)

PCA

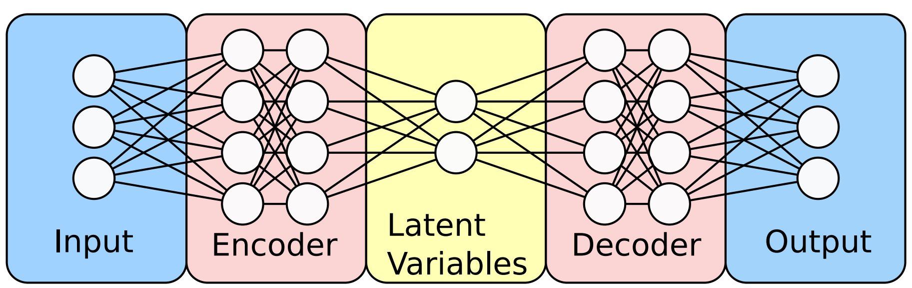


L. Wang, Phys. Rev. B
94, 195105 (2016)

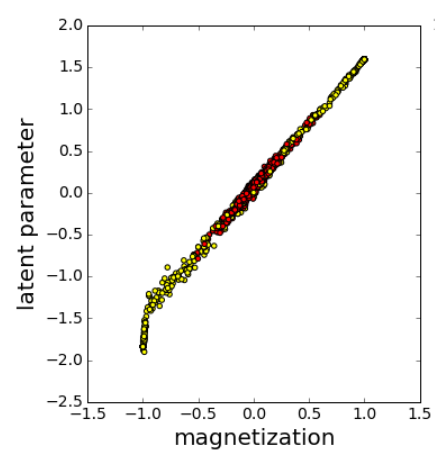
PCA



Nieuwenburg, Liu, and
Huber, Nat. Phys. (2017)

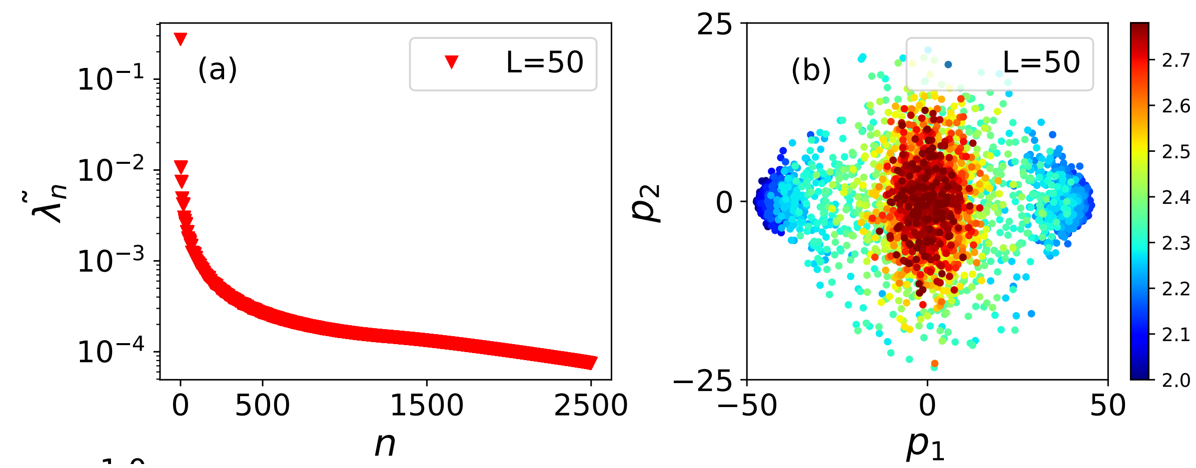


PCA / AE



S. J. Wetzel,
arXiv:1703.02435

PCA / AE



W. Hu, R. R.P. Singh, R. T. Scalettar,
Phys. Rev. E **95**, 062122 (2017)

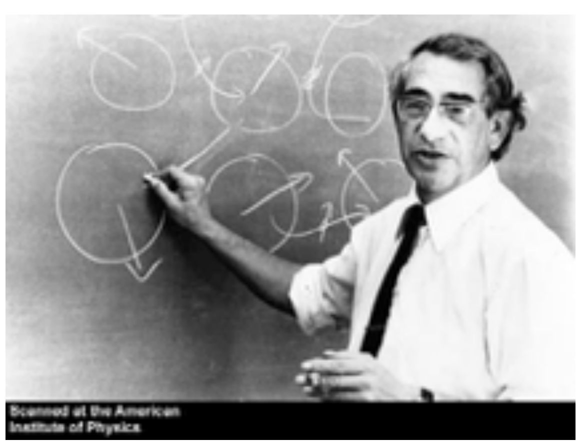
Can we do this for quantum systems?

The Fermi-Hubbard Model

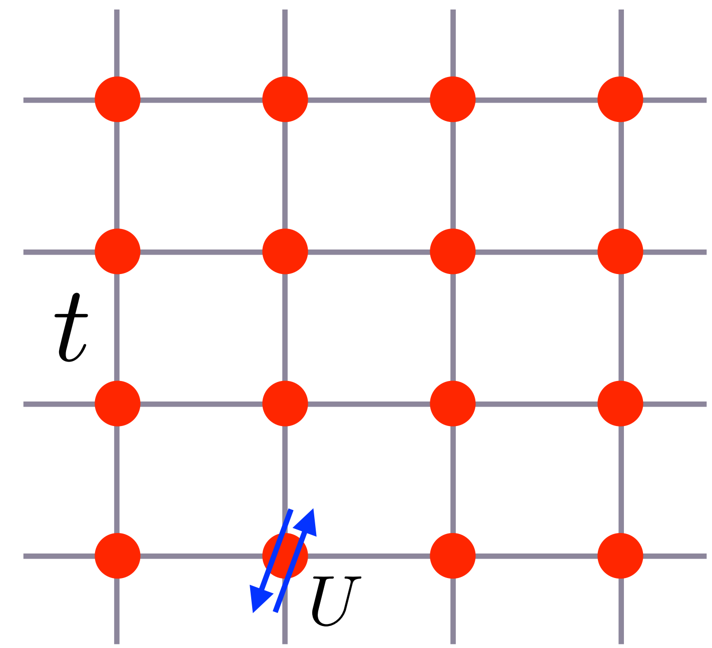
$$H = t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Enrico Fermi

John Hubbard



- Simple form
- Difficult to solve
- Rich physics:
  - Can tune U/t
  - Or vary the density
  - Quantum magnetism
  - Believed to have superconductivity
  - …



Average of one electron per site

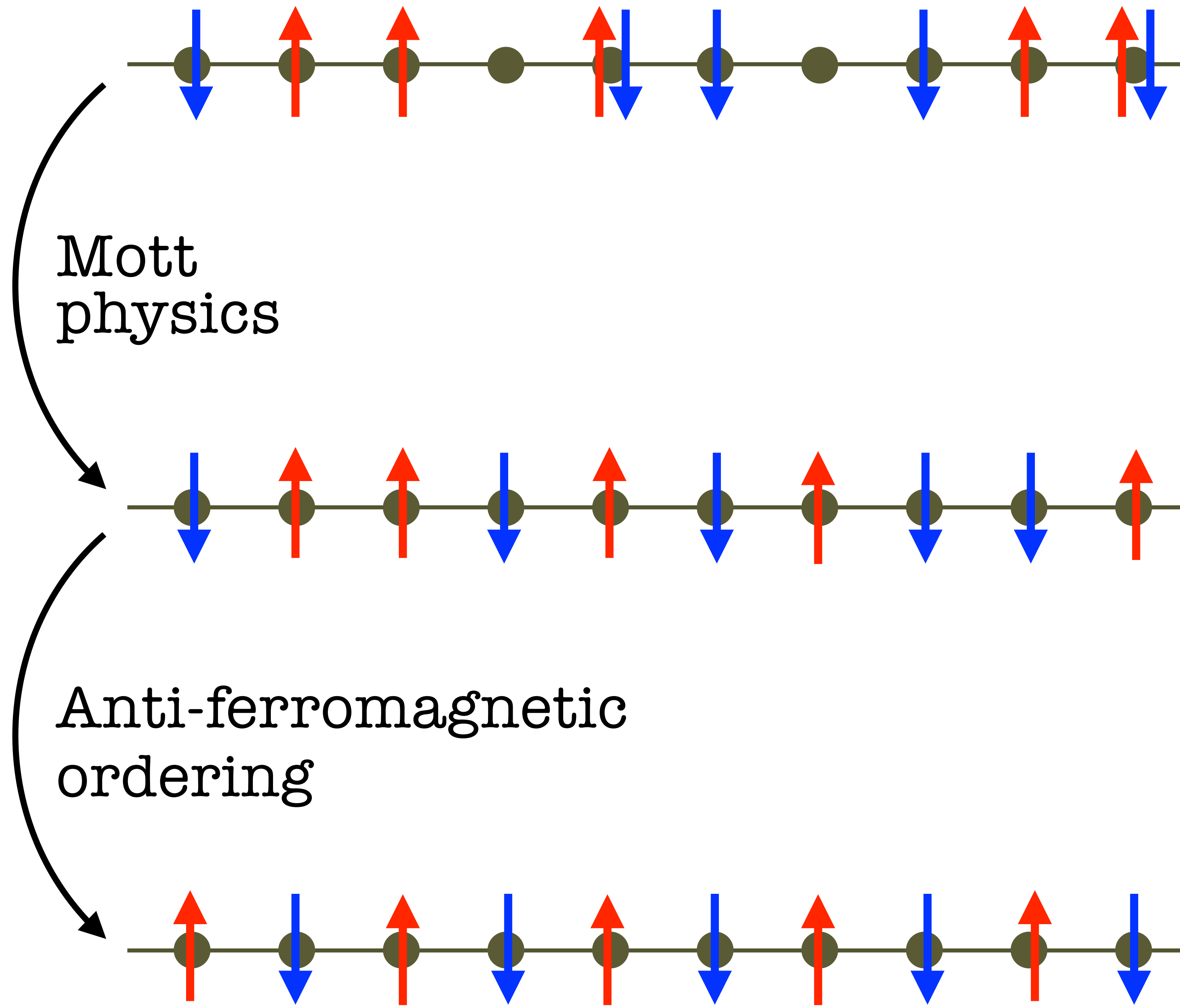
Decreasing Temperature

Random:

Suppressing charge degrees of freedom:

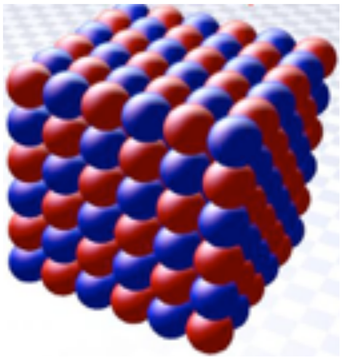
Effectively the Heisenberg model:

$$\hat{H} = J \sum_{ij} \vec{S}_i \cdot \vec{S}_j$$

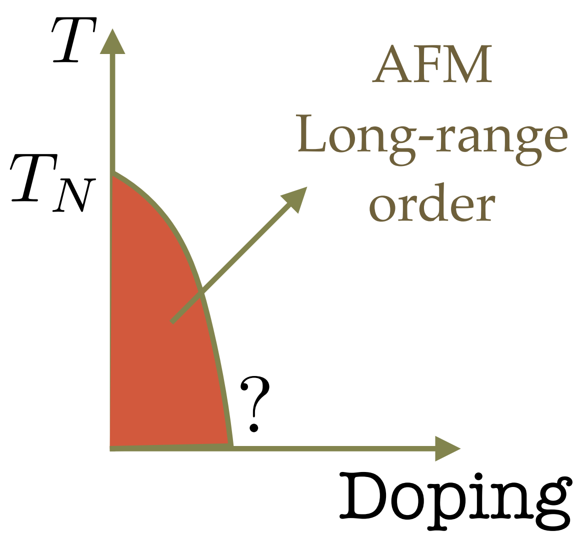


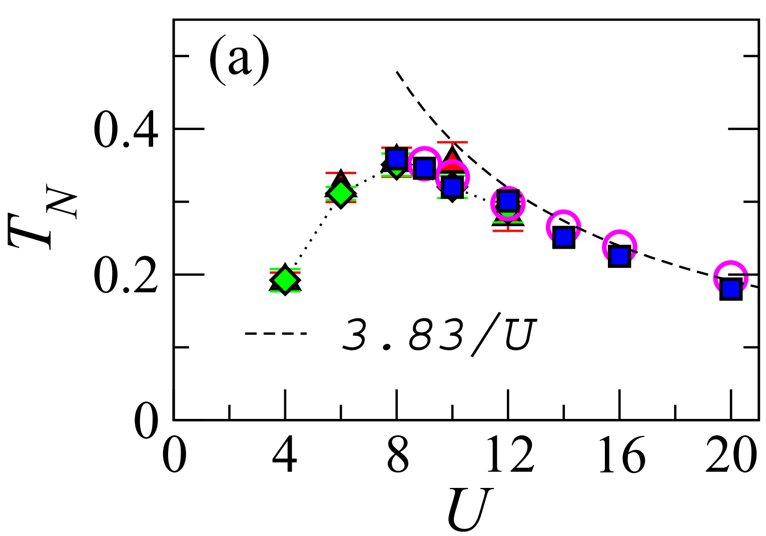
$$J = \frac{4t^2}{U}$$

3D Hubbard model at half filling

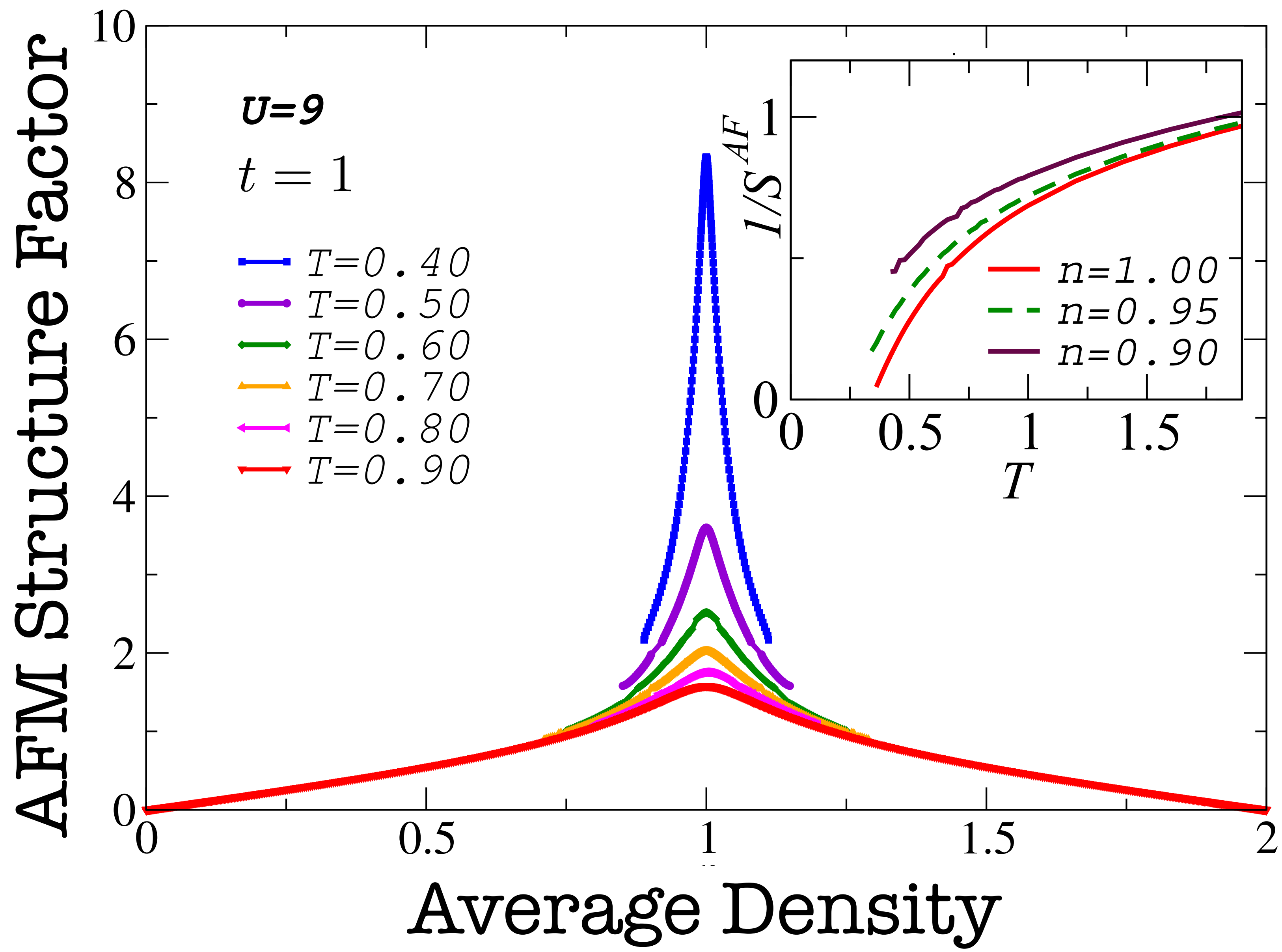


Hulet's group



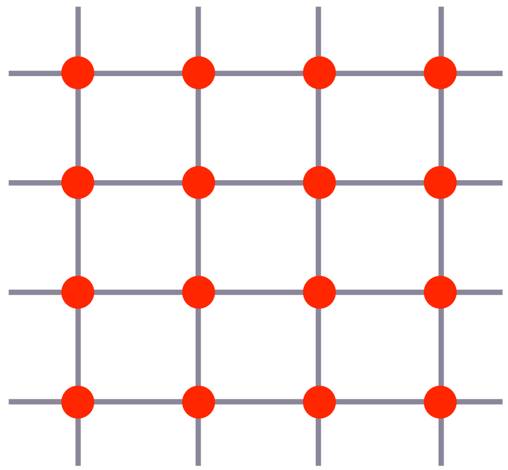


Finite-temperature magnetic phase transition in 3D.

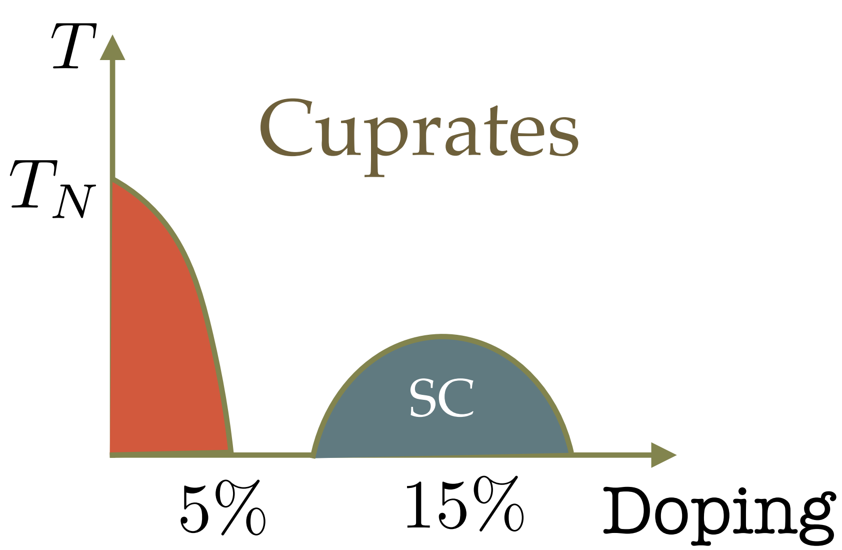


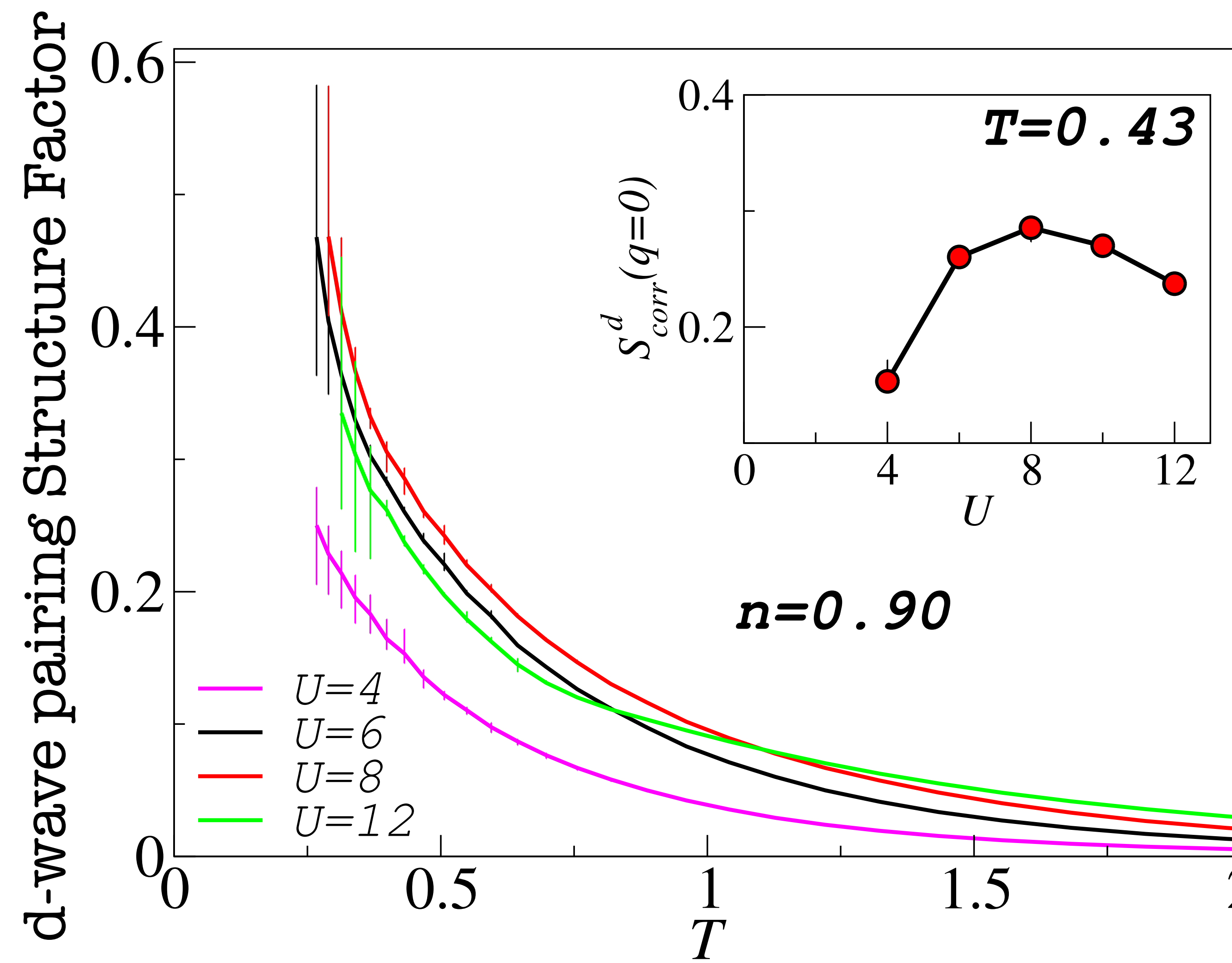
EK, Phys. Rev. B **94**, 125114 (2016)

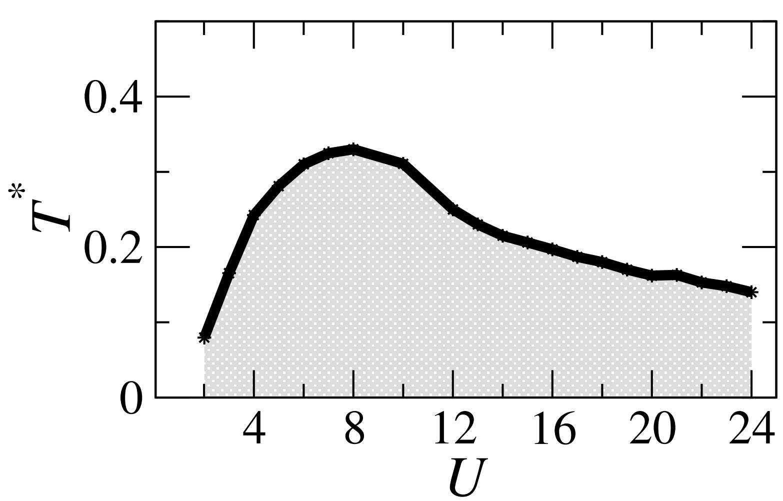
2D Hubbard model



No long-range magnetic order at finite temperatures!







EK, M. Rigol (2011)

EK, R. Scalettar, and R. R. P. Singh (2014)

Quantum Monte Carlo

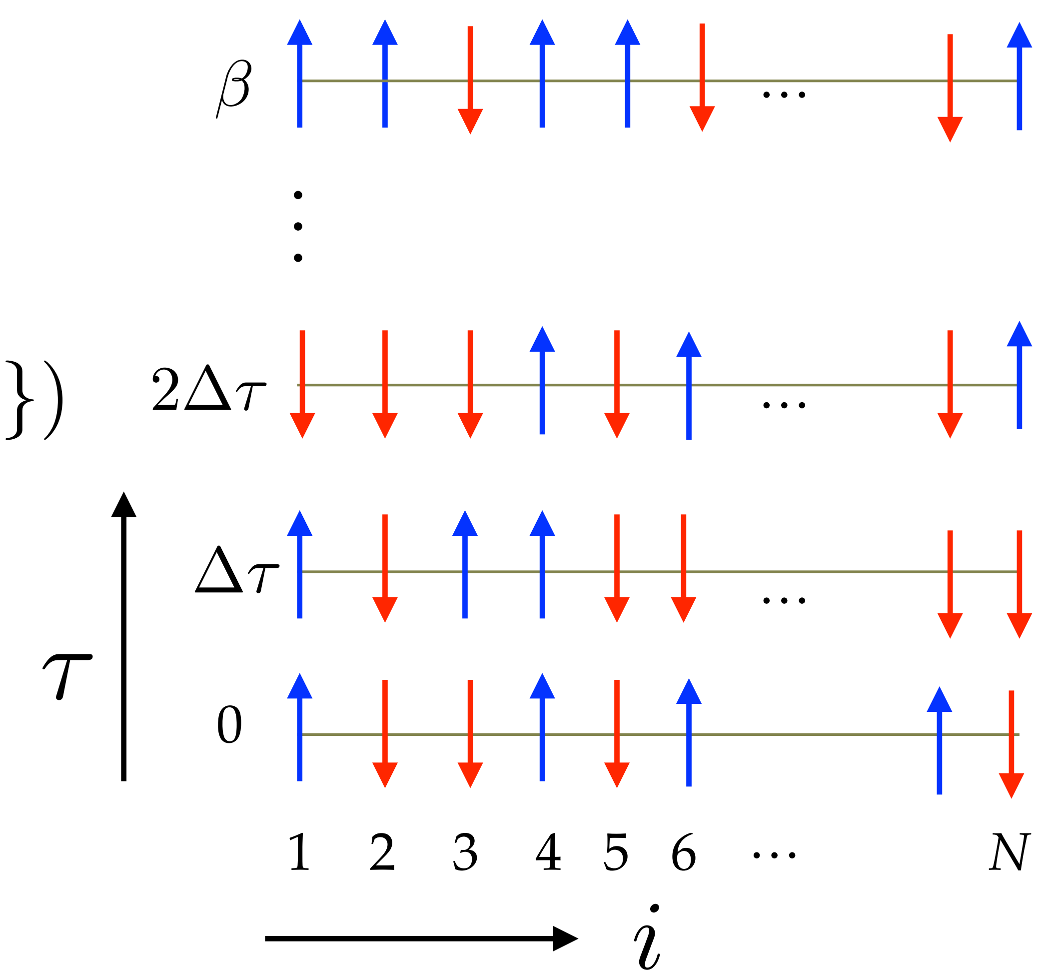
$$Z = \mathrm{Tr}e^{-\beta\hat{H}} = \mathrm{Tr}(e^{-\Delta\tau\hat{H}})^L \sim \mathrm{Tr}(e^{-\Delta\tau\hat{K}}e^{-\Delta\tau\hat{P}})^L \qquad \Delta\tau = \frac{\beta}{L}$$

$$e^{\Delta\tau U n_{i\uparrow}n_{i\downarrow}} = \frac{1}{2}\sum_{s_i=\pm1} e^{2\lambda s_i(n_{i\uparrow}-n_{i\downarrow})-\frac{\Delta\tau U}{2}(n_{i\uparrow}+n_{i\downarrow})}$$

Integrating out Fermionic degrees of freedom:

$$Z = \sum_{\{s_{i\tau}\}} \det M_{\uparrow}(\{s_{i\tau}\})\ \det M_{\downarrow}(\{s_{i\tau}\})$$

Sum taken stochastically over auxiliary variables that look like spins in d+1 dimensions!



Blankenbecler, R., Scalapino, D. J. & Sugar, R. L. Phys. Rev. D **24**, 2278 (1981)

Similar ideas in Broecker, Carrasquilla, Melko, and Trebst, arXiv:1608.07848

Sign Problem

$$Z = \sum_{\{s_{i\tau}\}} \det M_\uparrow(\{s_{i\tau}\}) \ \det M_\downarrow(\{s_{i\tau}\})$$

At half filling, both determinant have the same sign.

Away from half filling, our probability can become negative:
—-> "sign problem"

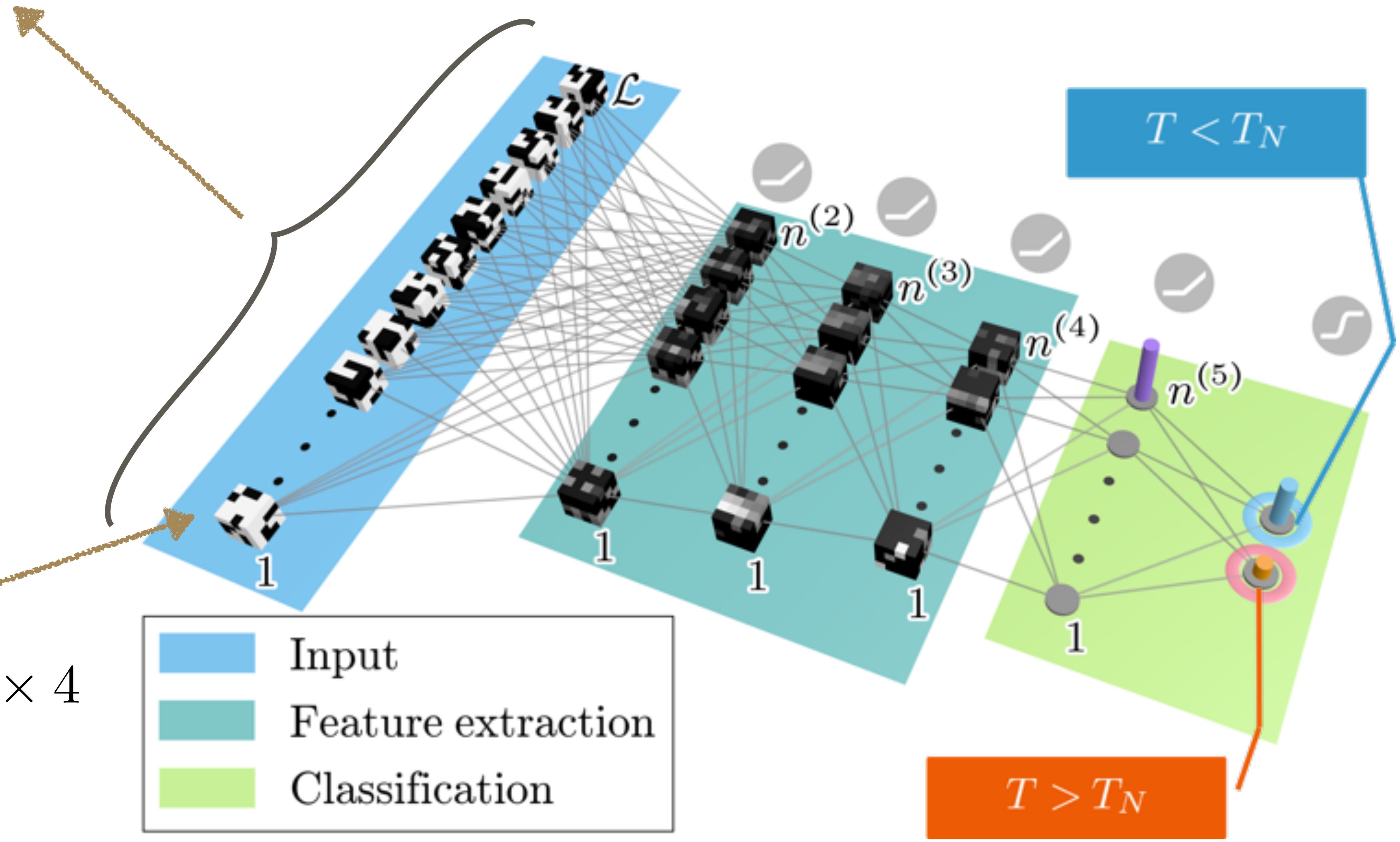
Can still estimate properties:

$$\langle O \rangle_p = \frac{\sum OP}{\sum P} = \frac{\sum O\mathcal{S}|P|}{\sum \mathcal{S}|P|} = \frac{\sum O\mathcal{S}|P| / \sum |P|}{\sum \mathcal{S}|P| / \sum |P|} = \frac{\langle\langle \mathcal{S}O \rangle\rangle_{|P|}}{\langle\langle \mathcal{S} \rangle\rangle_{|P|}}$$

Dividing two very small #s

A Convolutional Neural Network

$\mathcal{L} = 200$ # of time slices (color channels)



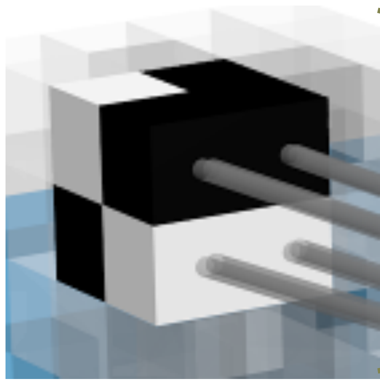
$N = 4 \times 4 \times 4$

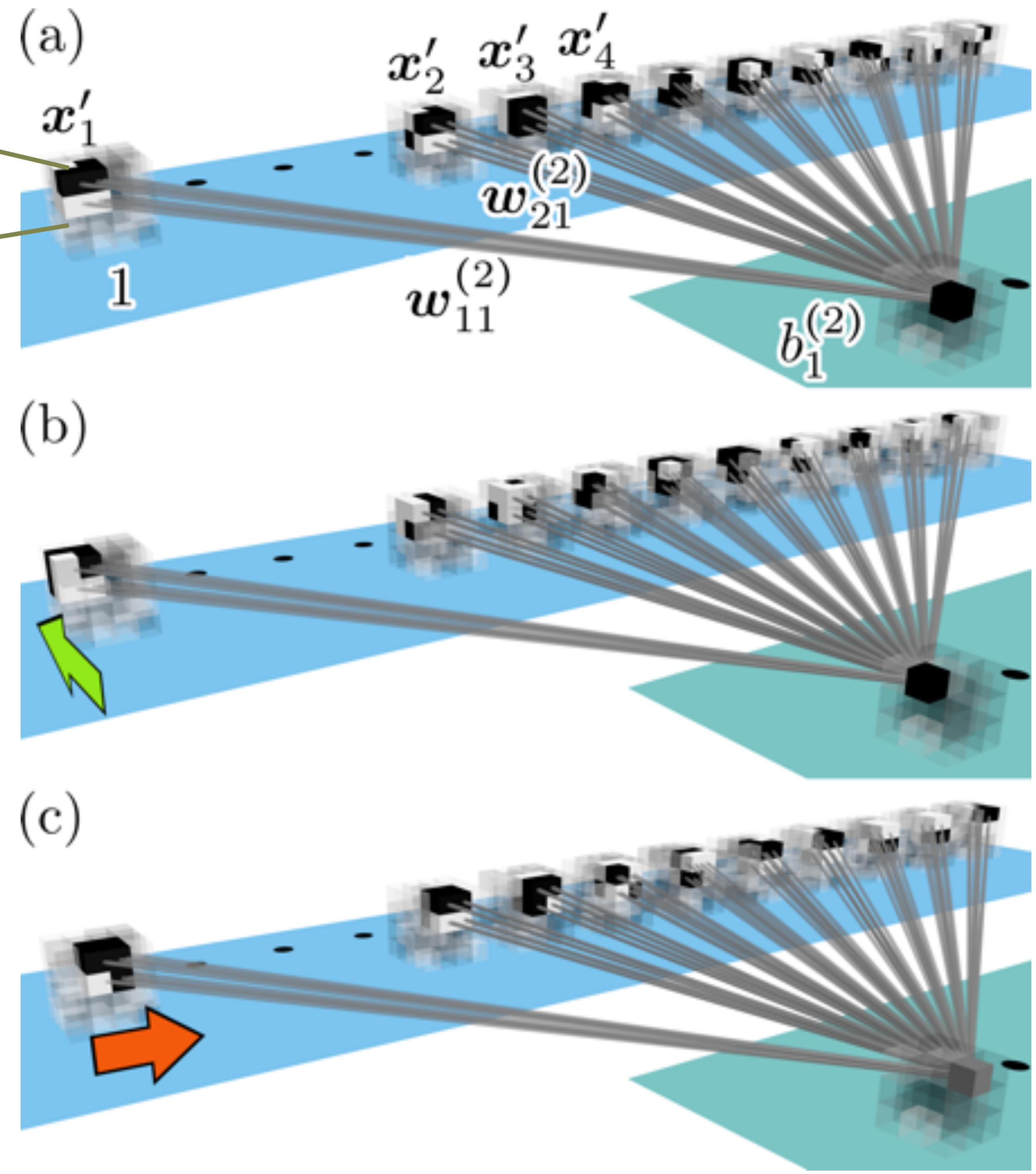
K. Ch'ng, J. Carrasquilla, R. G. Melko, EK, arXiv:1609.02552

TensorFlow

Convolutions

$2 \times 2 \times 2$ Fileter





$x'_l : 2 \times 2 \times 2$ **local input**

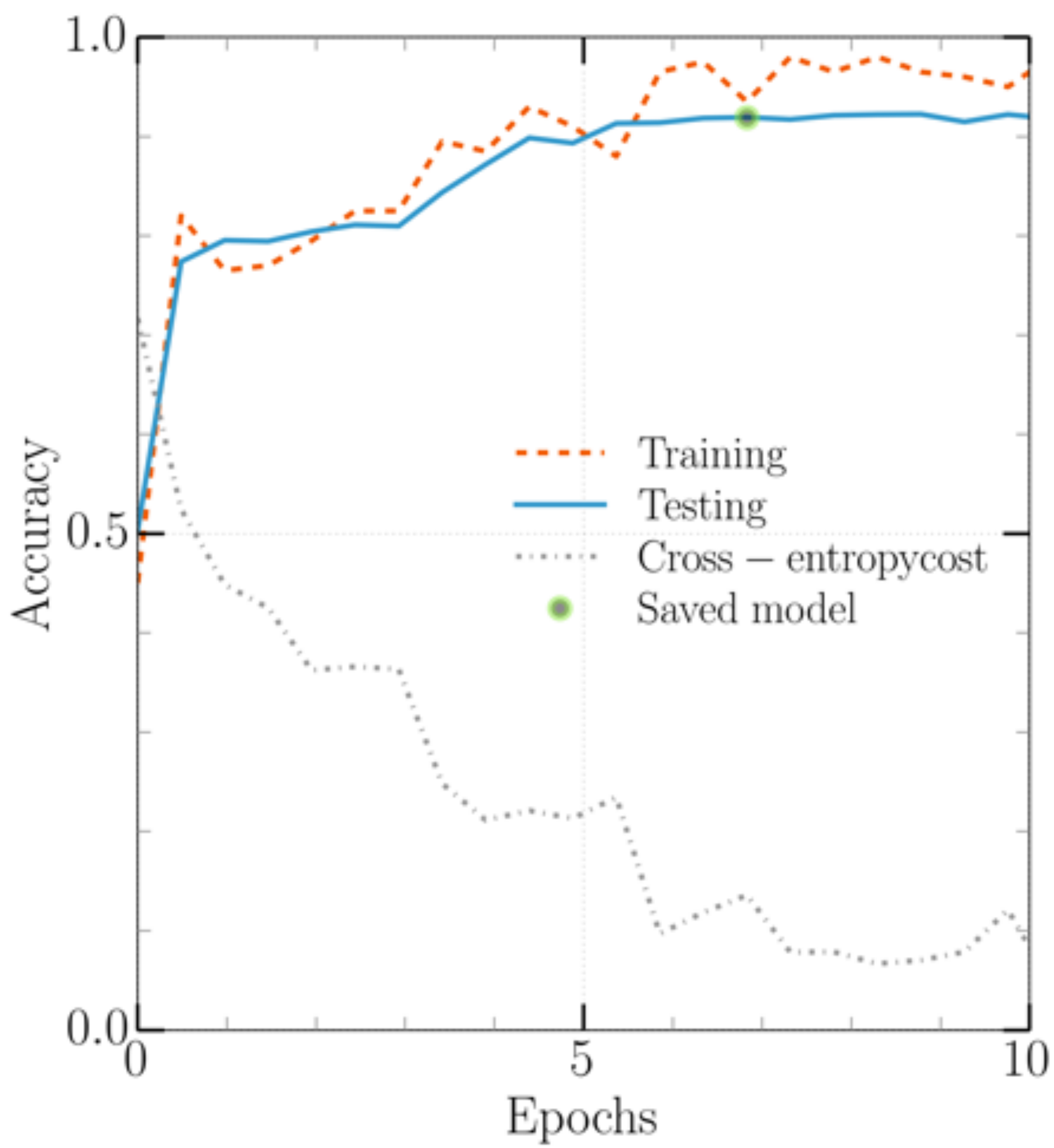
$w^{(2)}_{lm} : 2 \times 2 \times 2$ **volumetric filter**

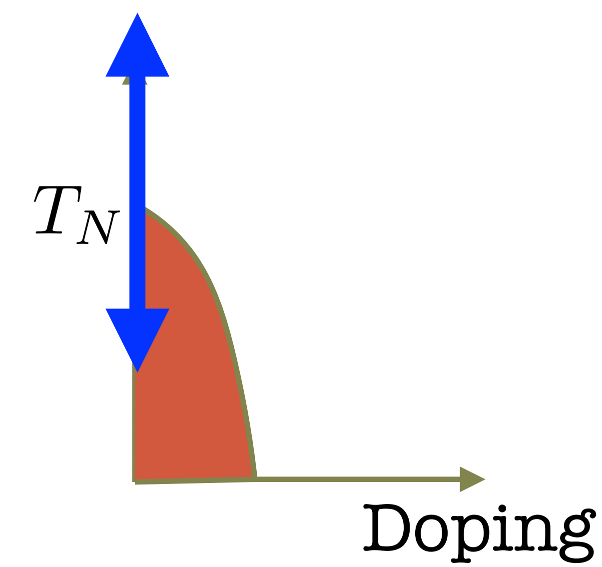
$$z_m = \sum_l \mathbf{w}^{(2)}_{lm} \cdot \mathbf{x}'_l + b^{(2)}_m$$

$$f = \max(0, z)$$

Training

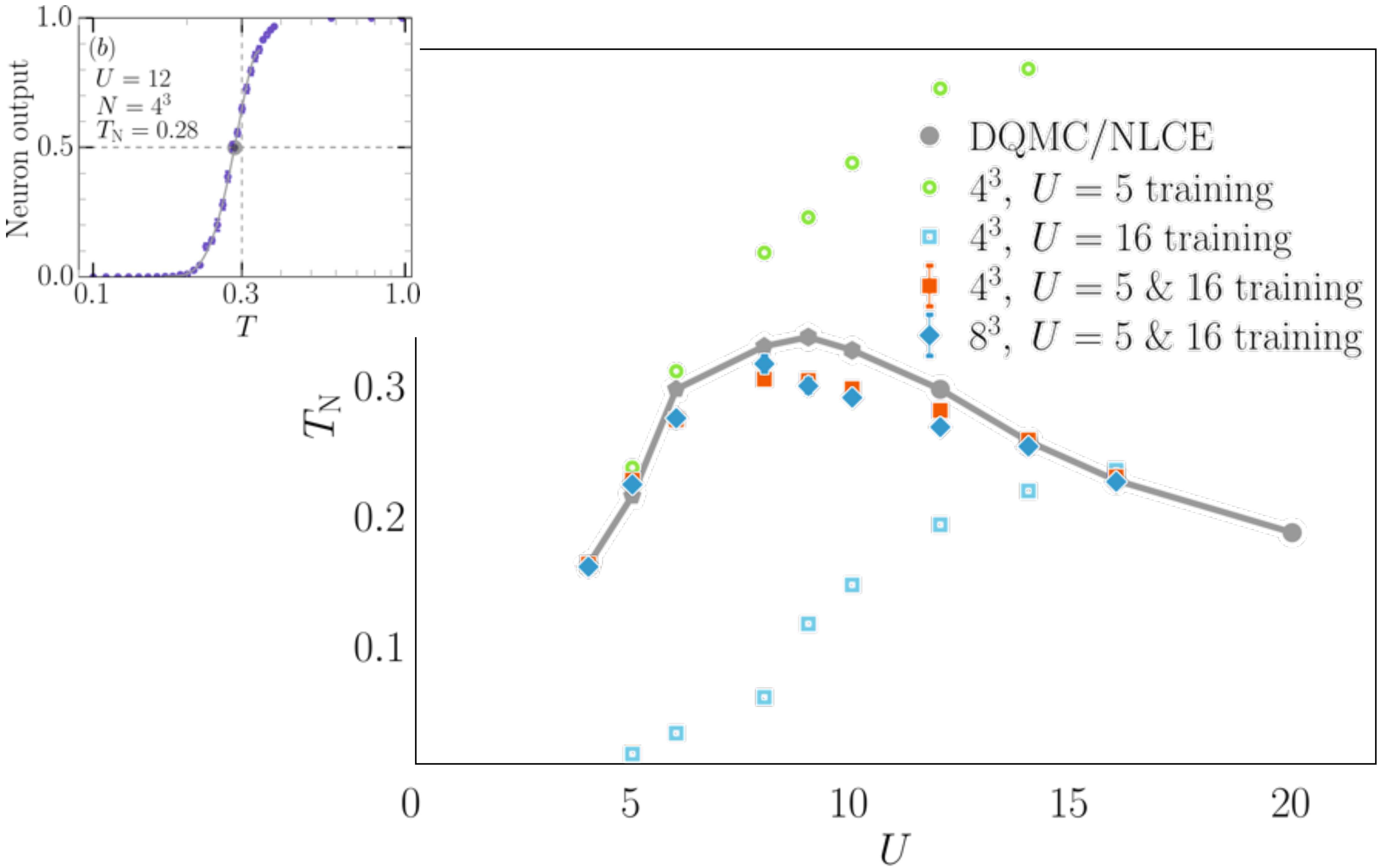
Use labeled auxiliary spin configuration over a range of temperatures at half filling for a fixed U





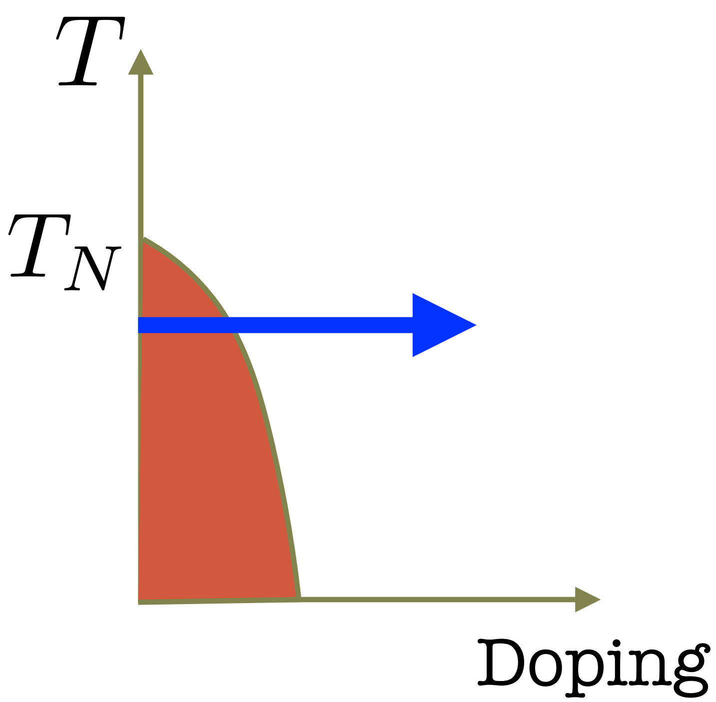
1. Load 85 % of data for training and 15 % for unbiased testing.
2. Small batch of data is used for computing gradient through backbackpagation of error.
3. w and b are adjusted.

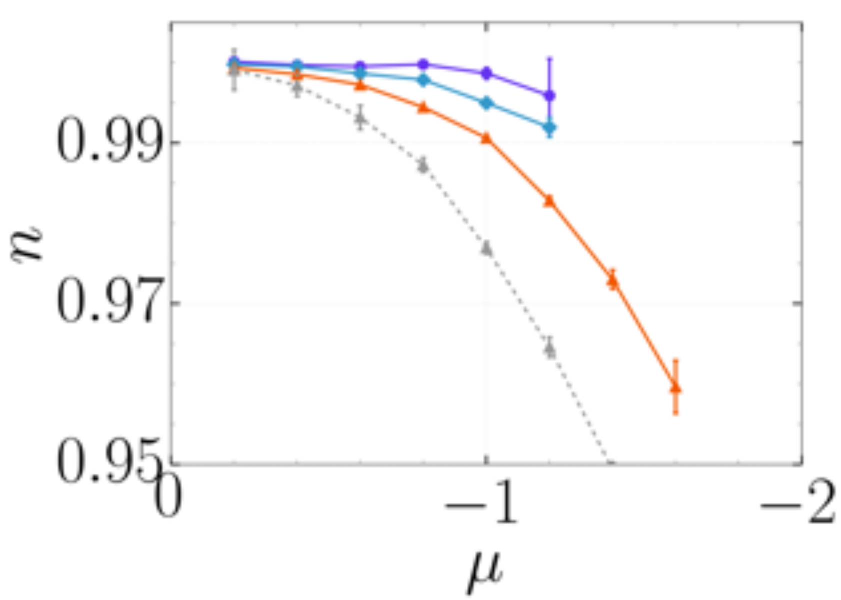
Predicting The Neel Temperature



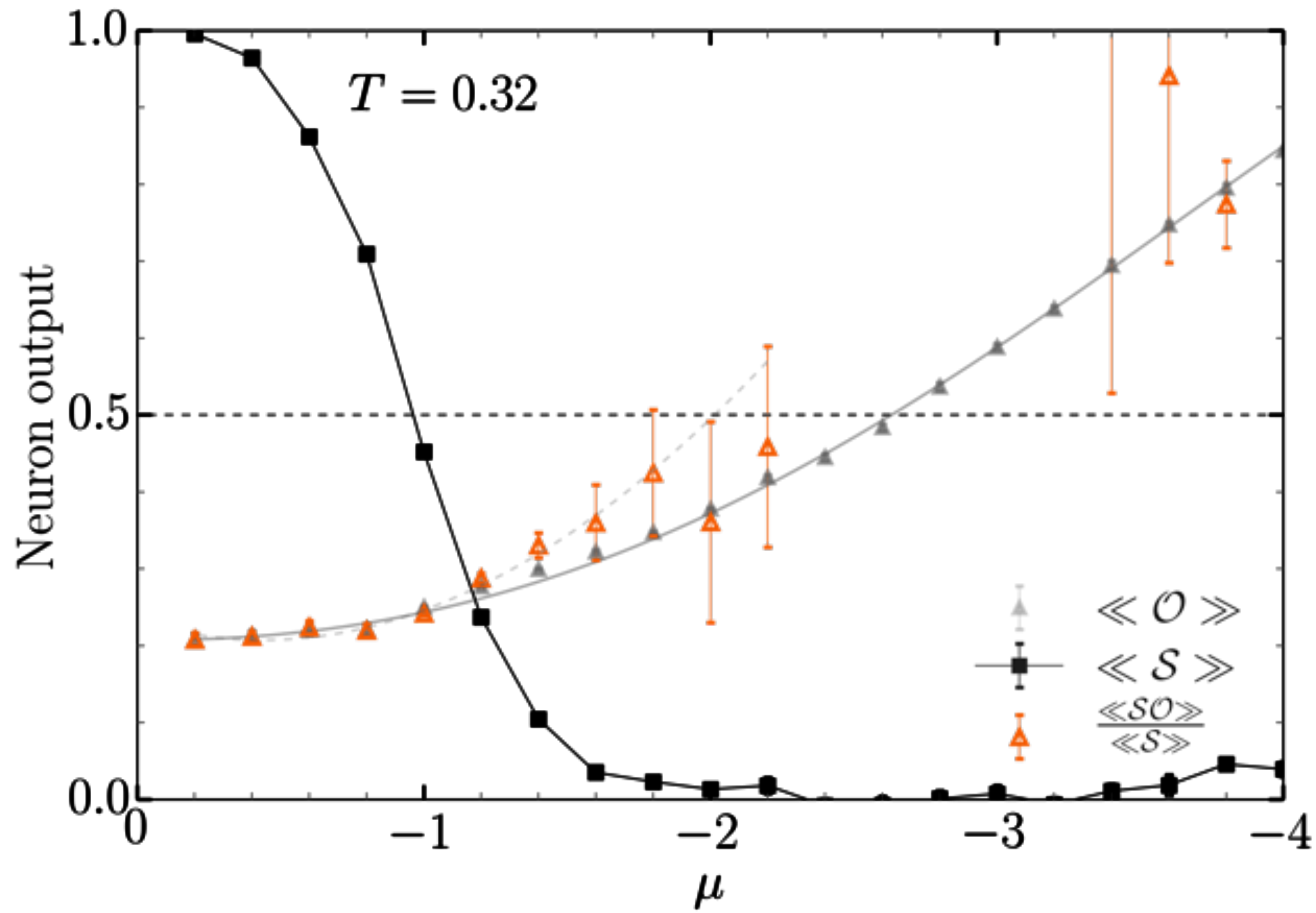
K. Ch'ng, J. Carrasquilla, R. G. Melko, EK, arXiv:1609.02552

Away From Half Filling



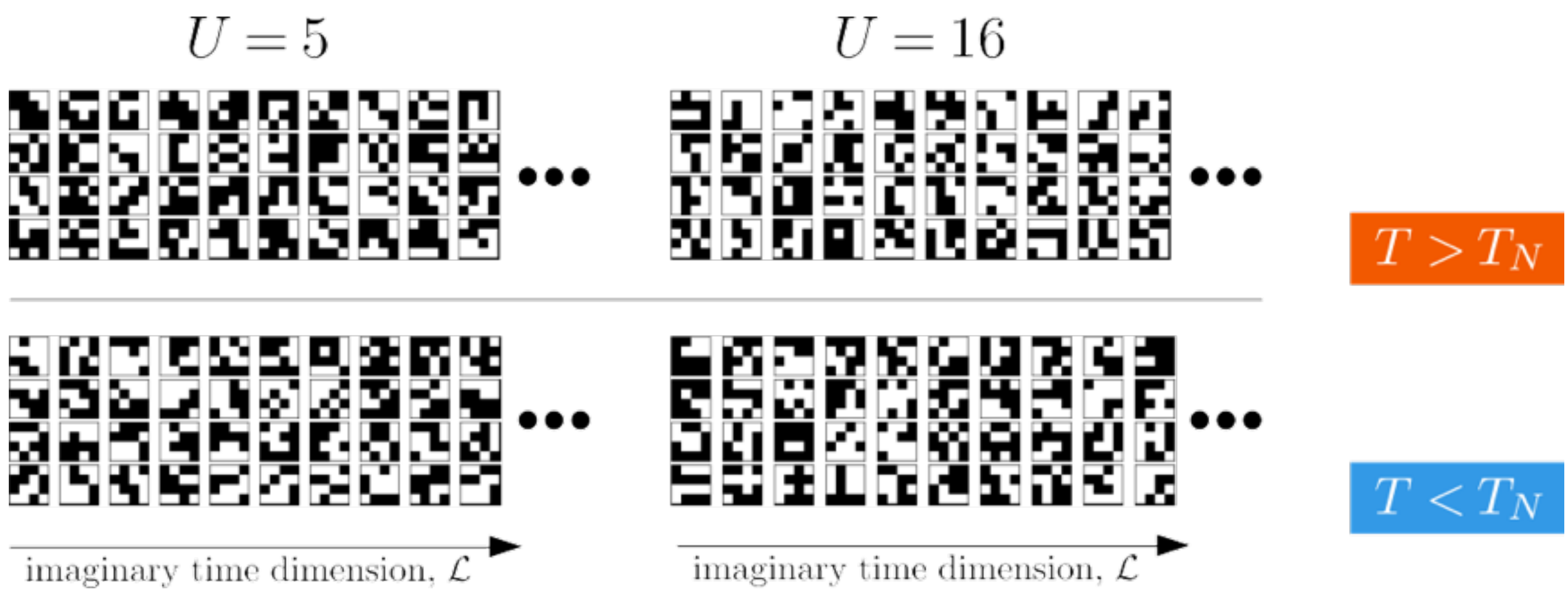


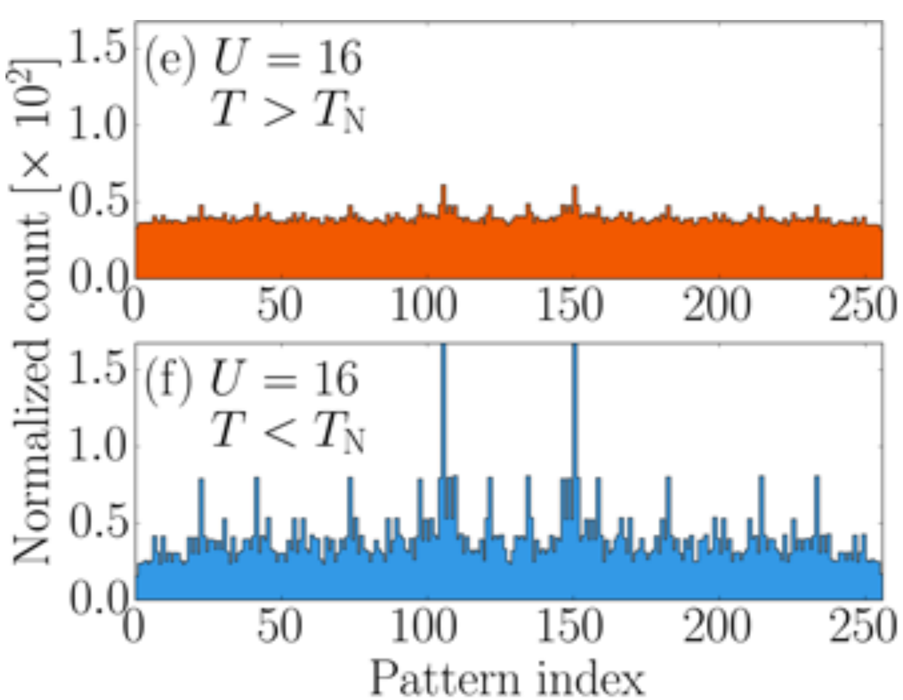
Transfer learning from half filling

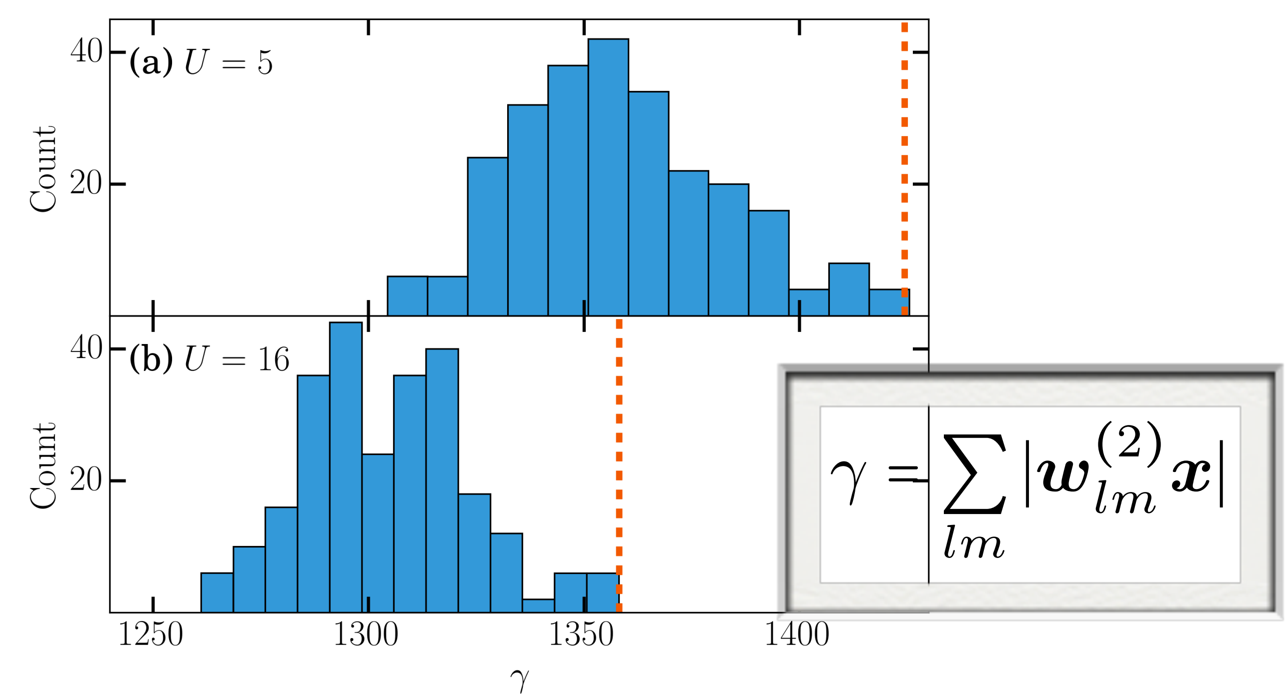


K. Ch'ng, J. Carrasquilla, R. G. Melko, EK, arXiv:1609.02552

What Has the Machine Learned?

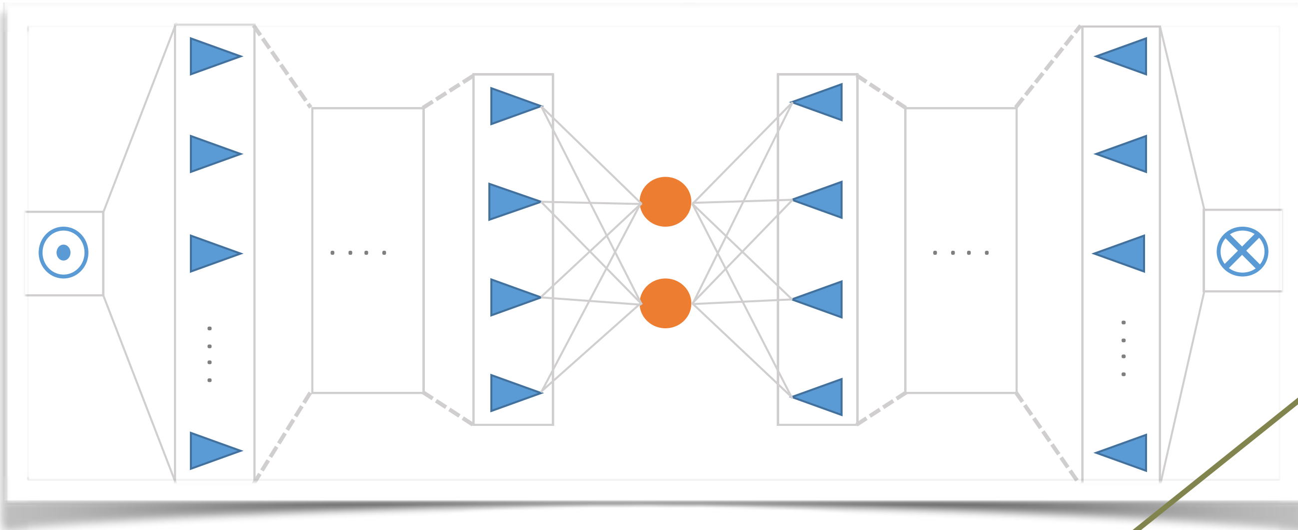






What About Unsupervised ML?

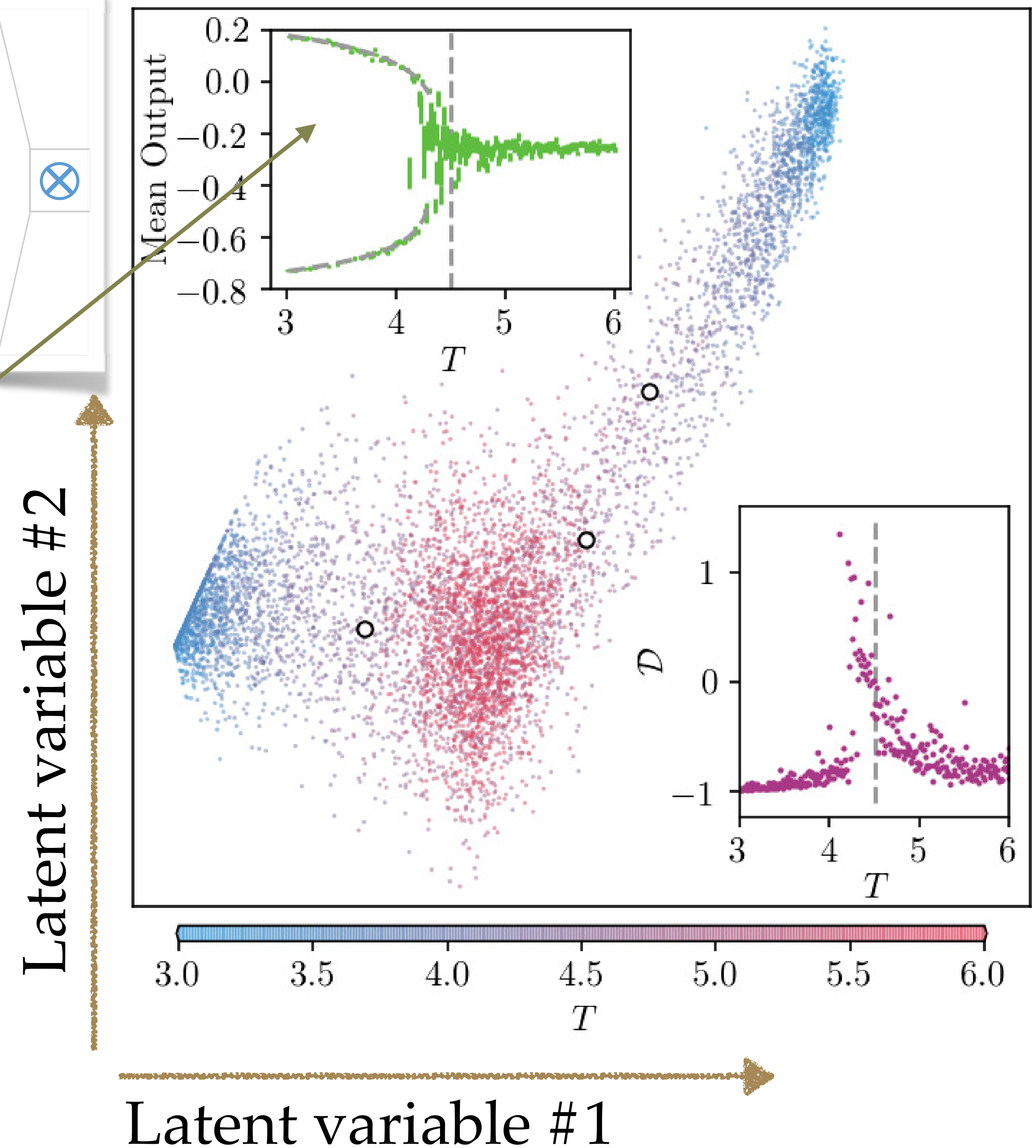
Conv. Autoencoder: 3D Ising Model



$T_N \sim 4.5J$

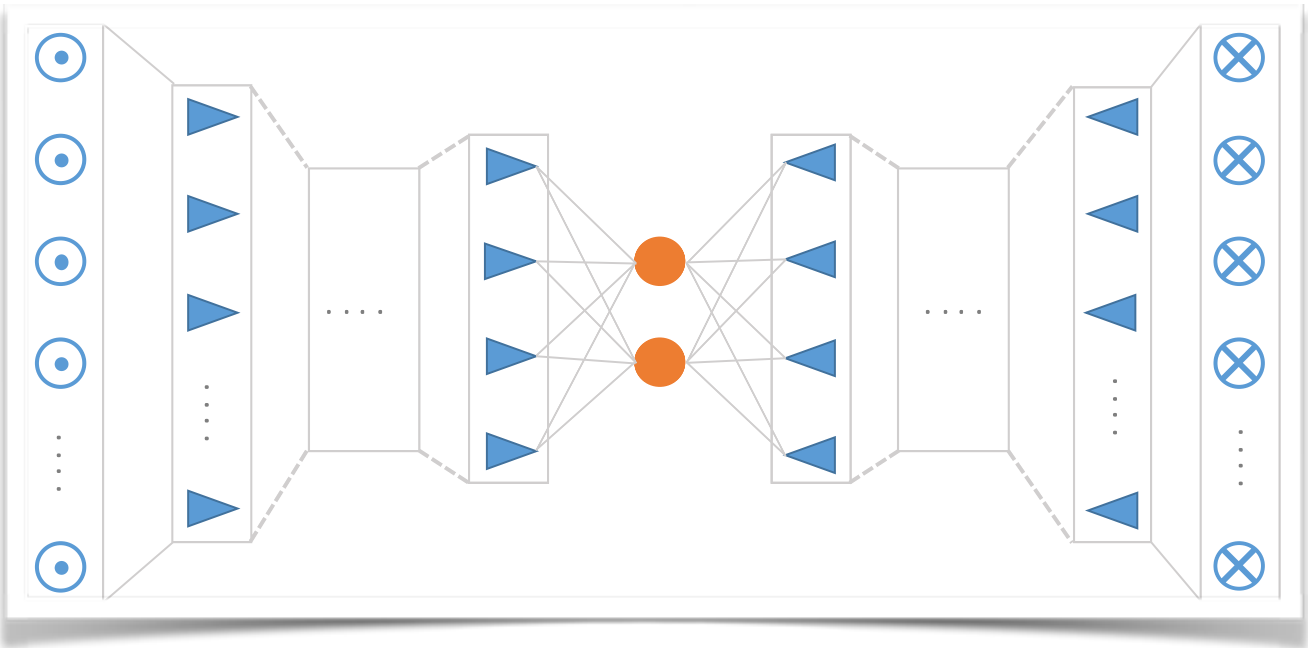
Consistent with
fit to output of single
latent variable with
critical exponent

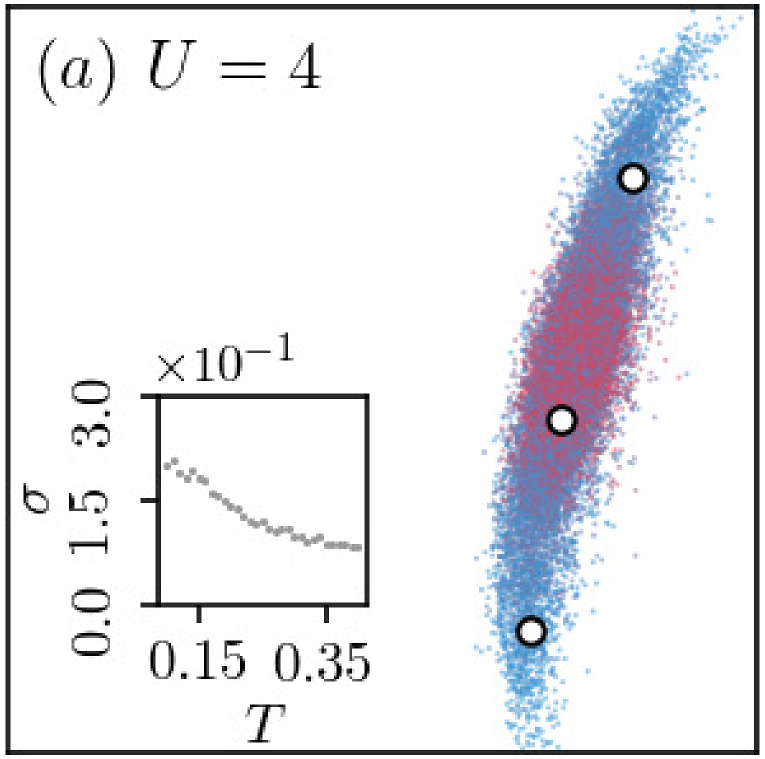
$\beta = 0.34$



Conv. Autoencoder: 3D Hubbard Model

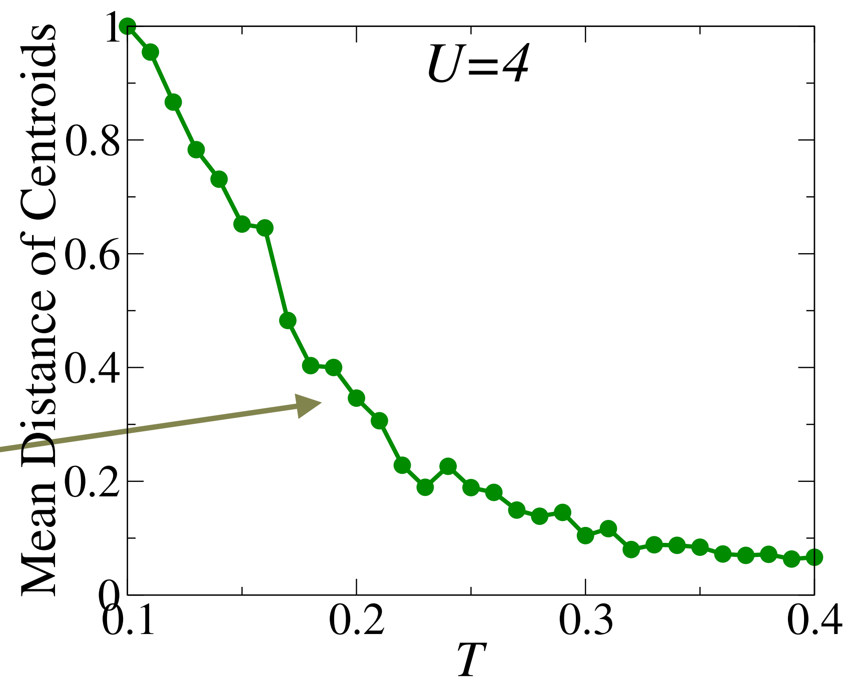
One input cube per time slice:



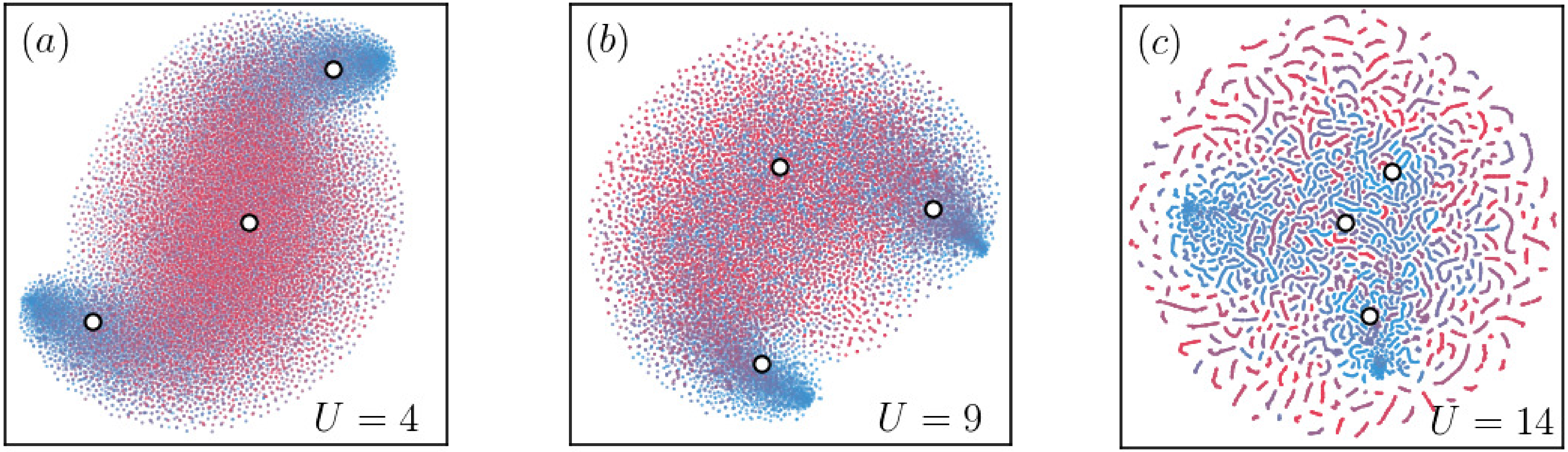


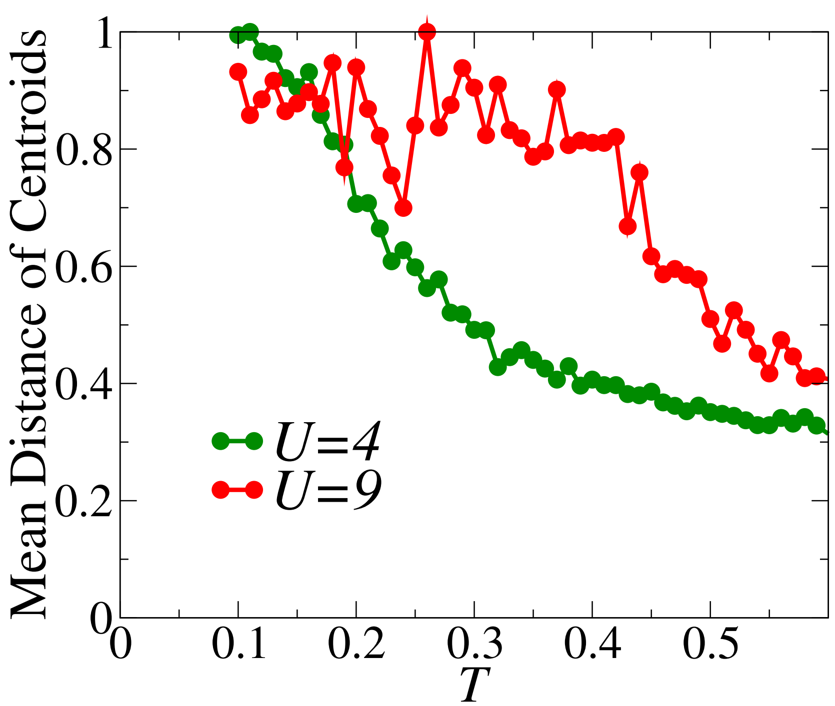
No perfect separation for the quantum case!

Sharpest rise of the indicator around the expected critical temperature ~0.2

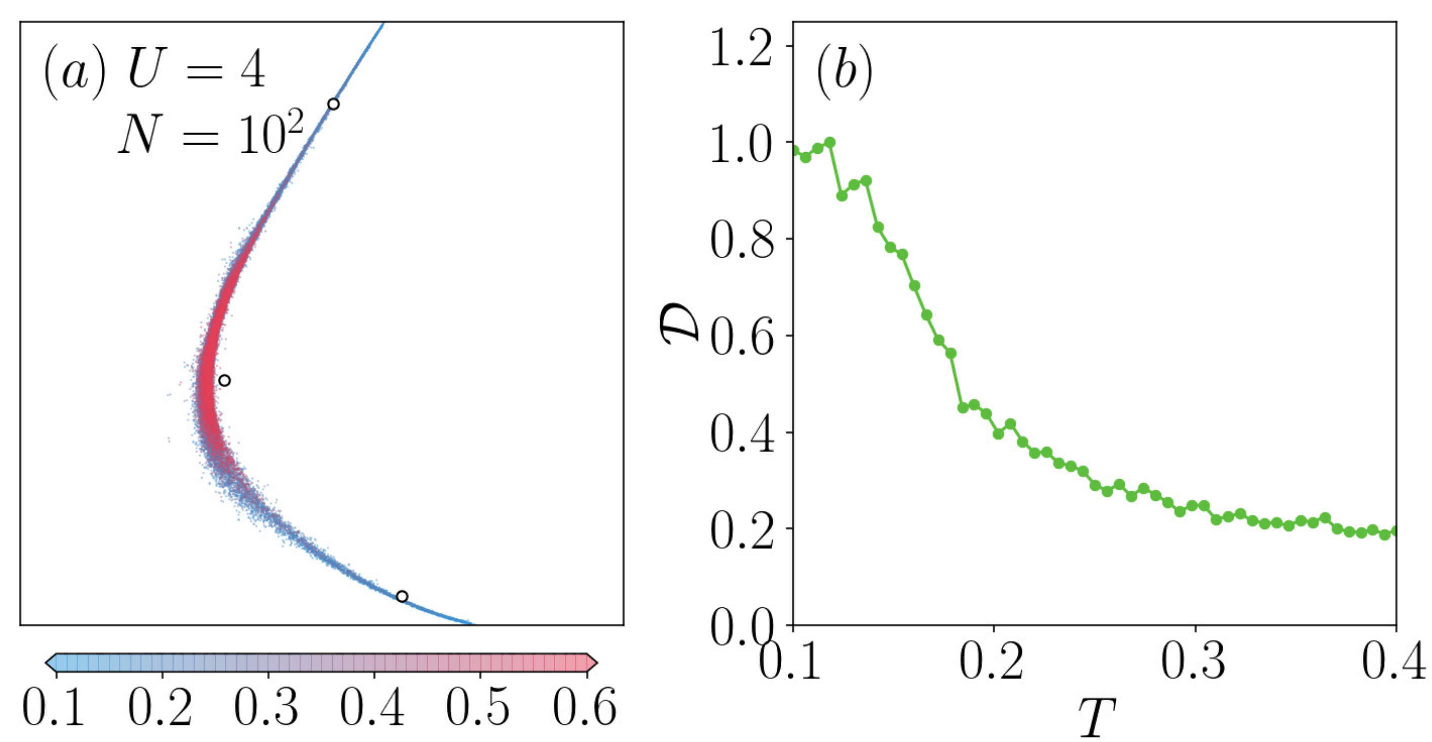


t_SNE: Hubbard Models



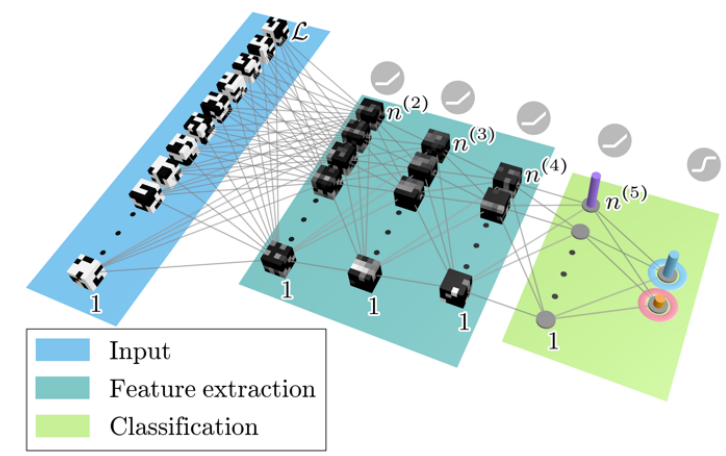


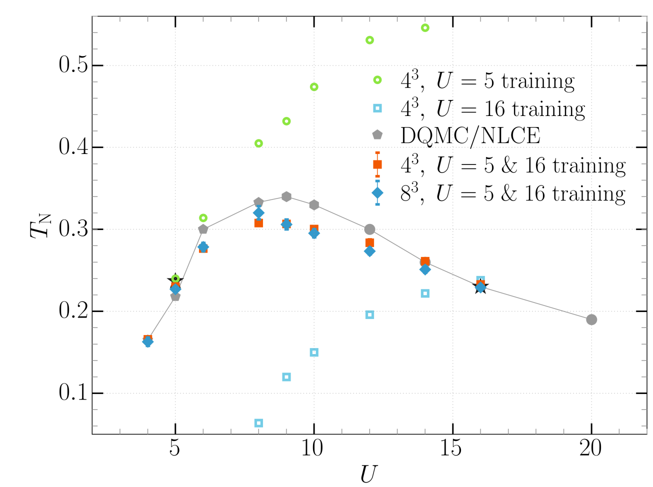
2D Hubbard



Summary

- Using a 3D CNN, we are able to predict magnetic critical temperature of the Fermi-Hubbard model as the interaction is varied.





- Unsupervised ML techniques can be used for quantum systems, however, it is hard to extract meaningful indicators for critical behavior similar to classical models.