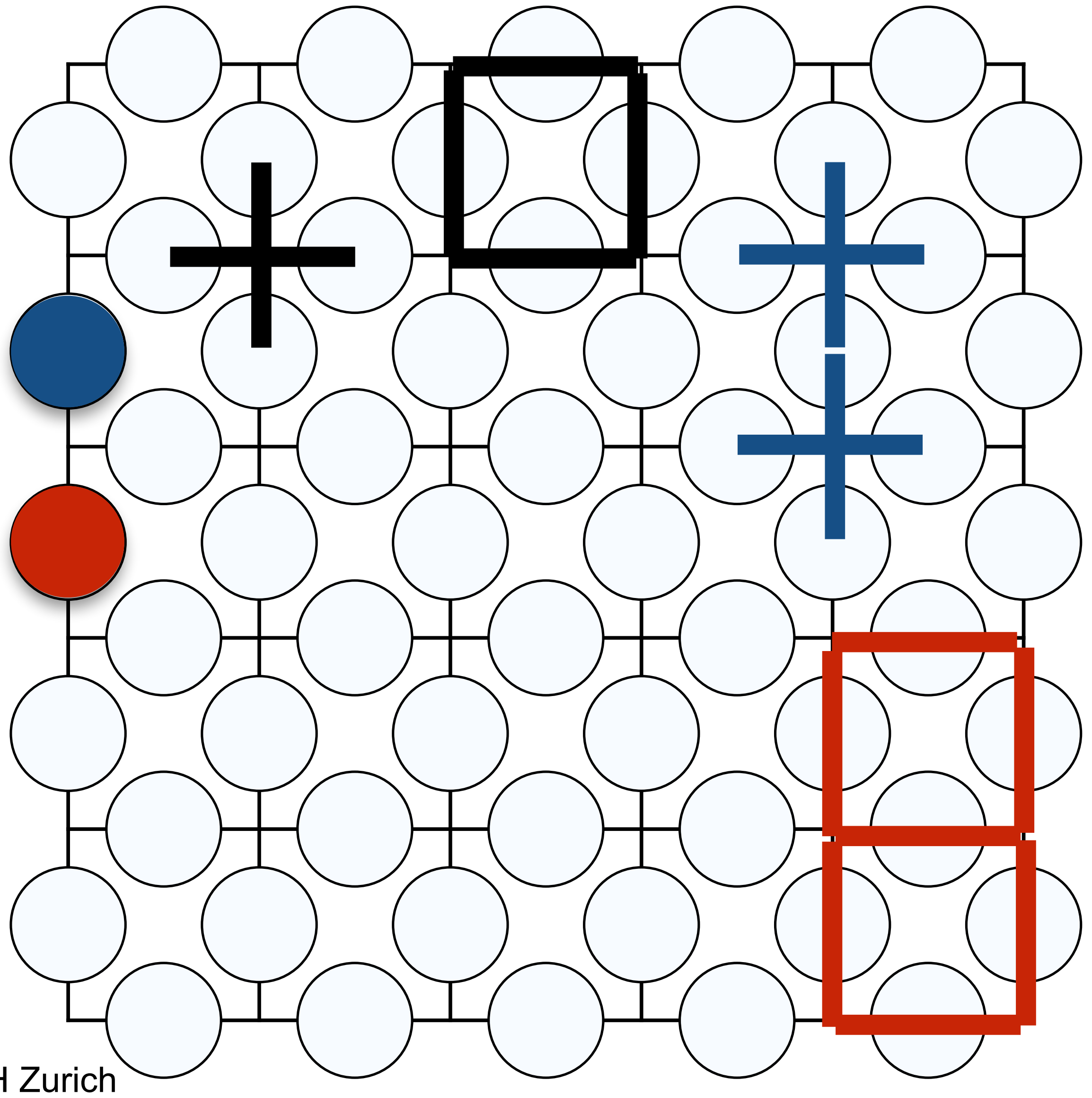
Predicting Phase Transitions in Many-Body Physics

arXiv: 1910.10124

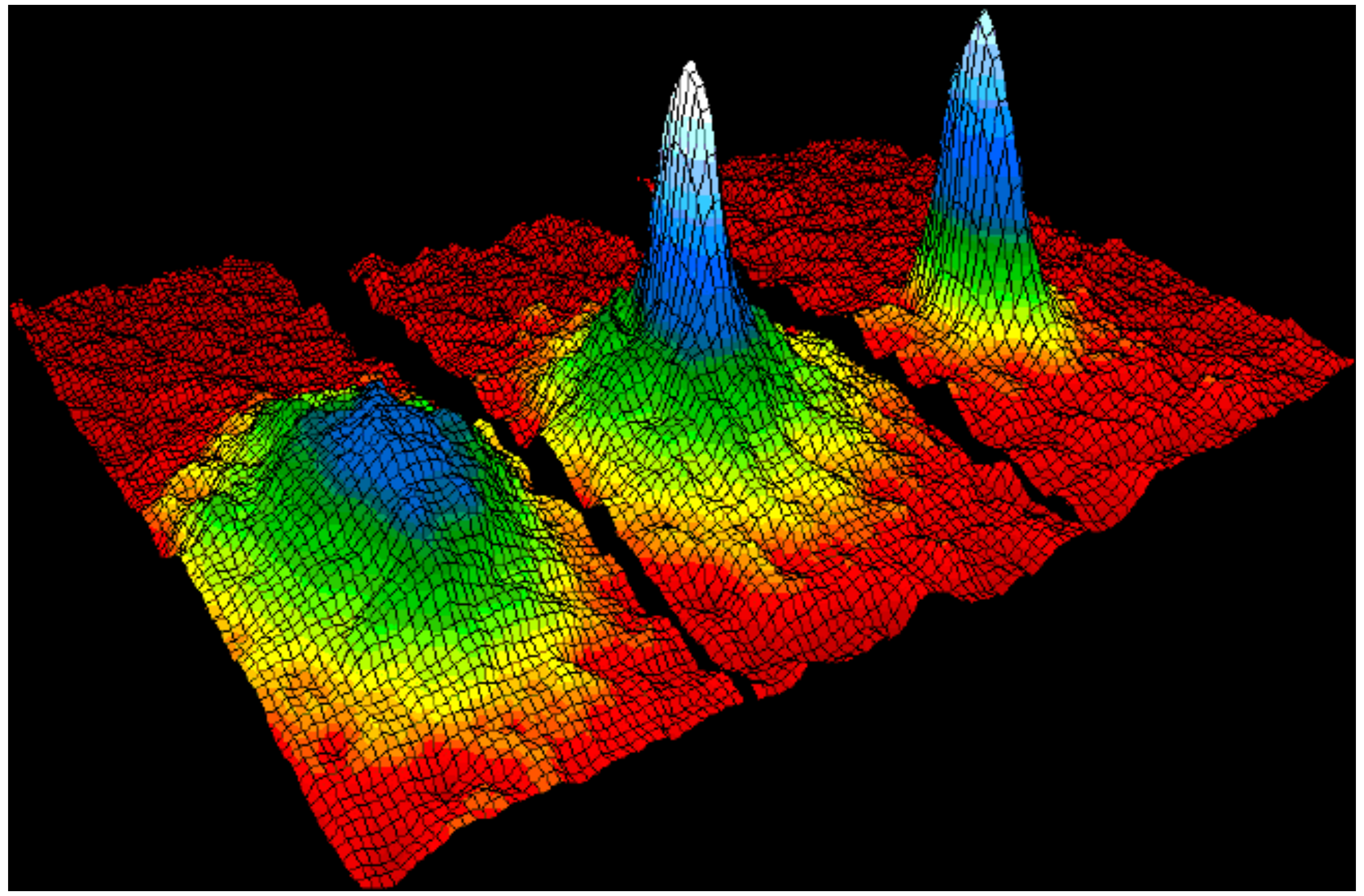
Eliška Greplová, ETH Zürich

Phase transitions

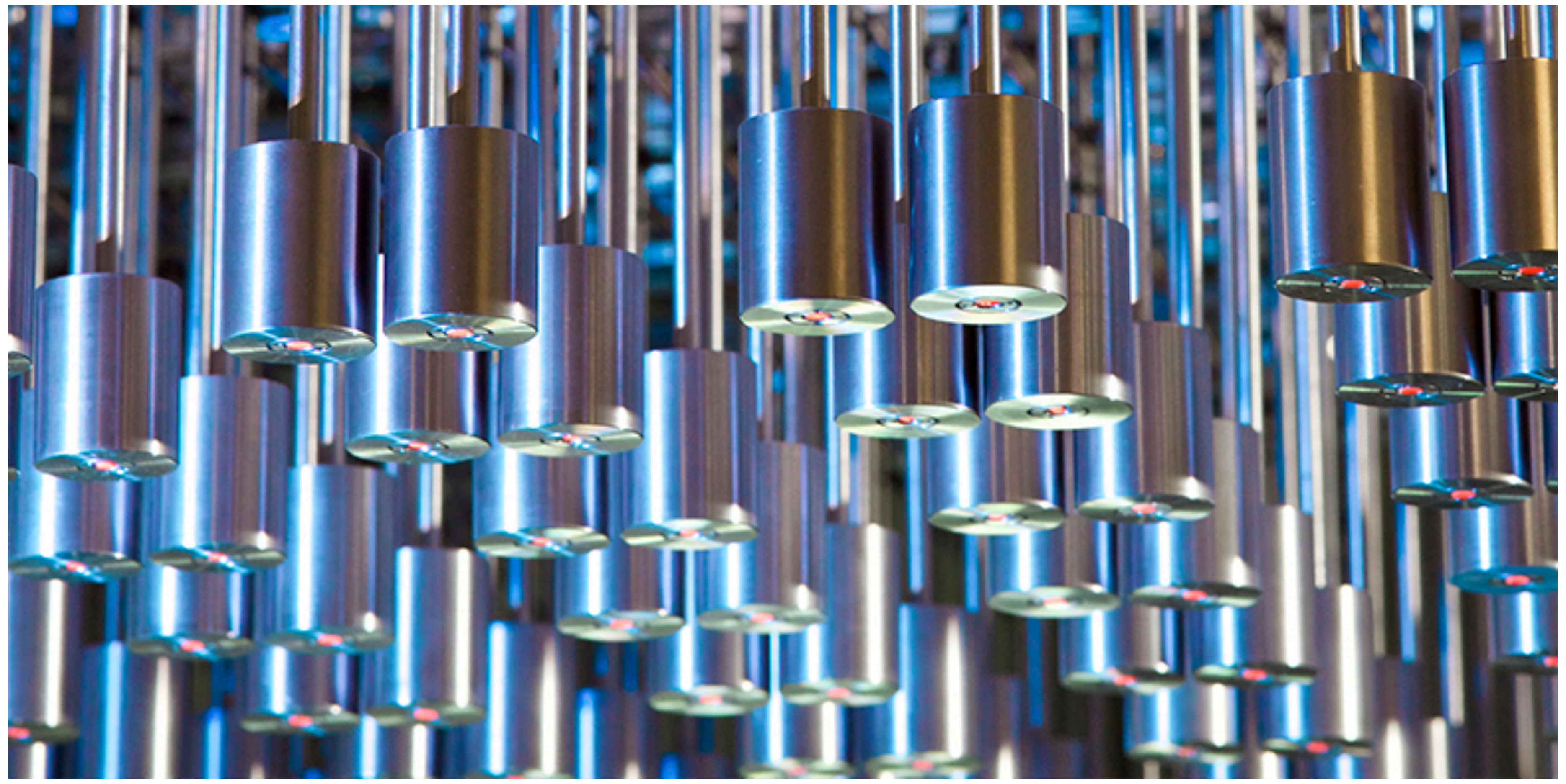
Zaria Forman



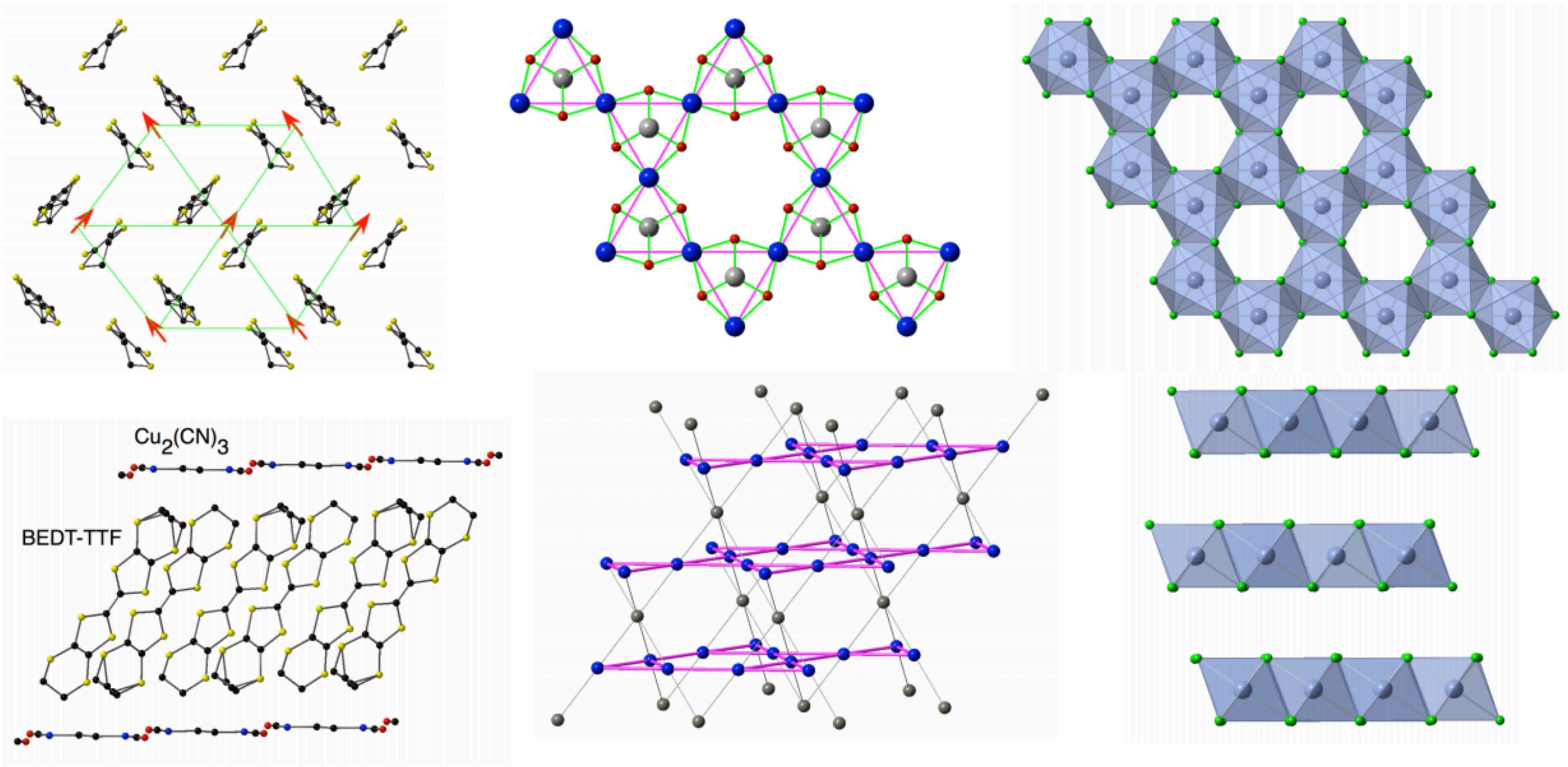
ETH Zurich



NIST/JILA/CU-Boulder



ETH Zurich



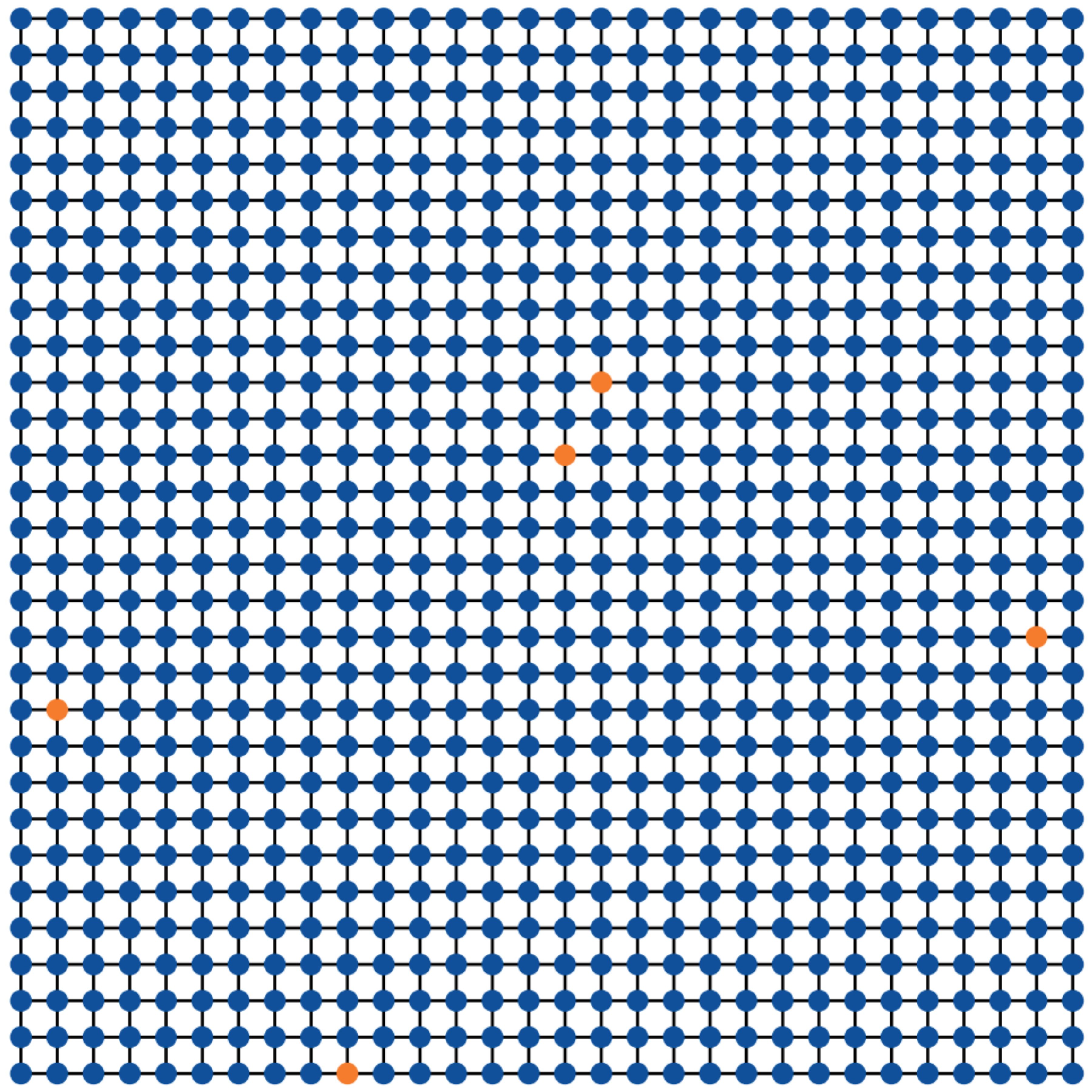
arXiv: 1905.07040

Can we understand critical behaviour in condensed matter just via analysis of measured data?

Simple Example: Ising Model

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j$$

temperature-driven phase transition:
ferromagnetic -> paramagnetic phase

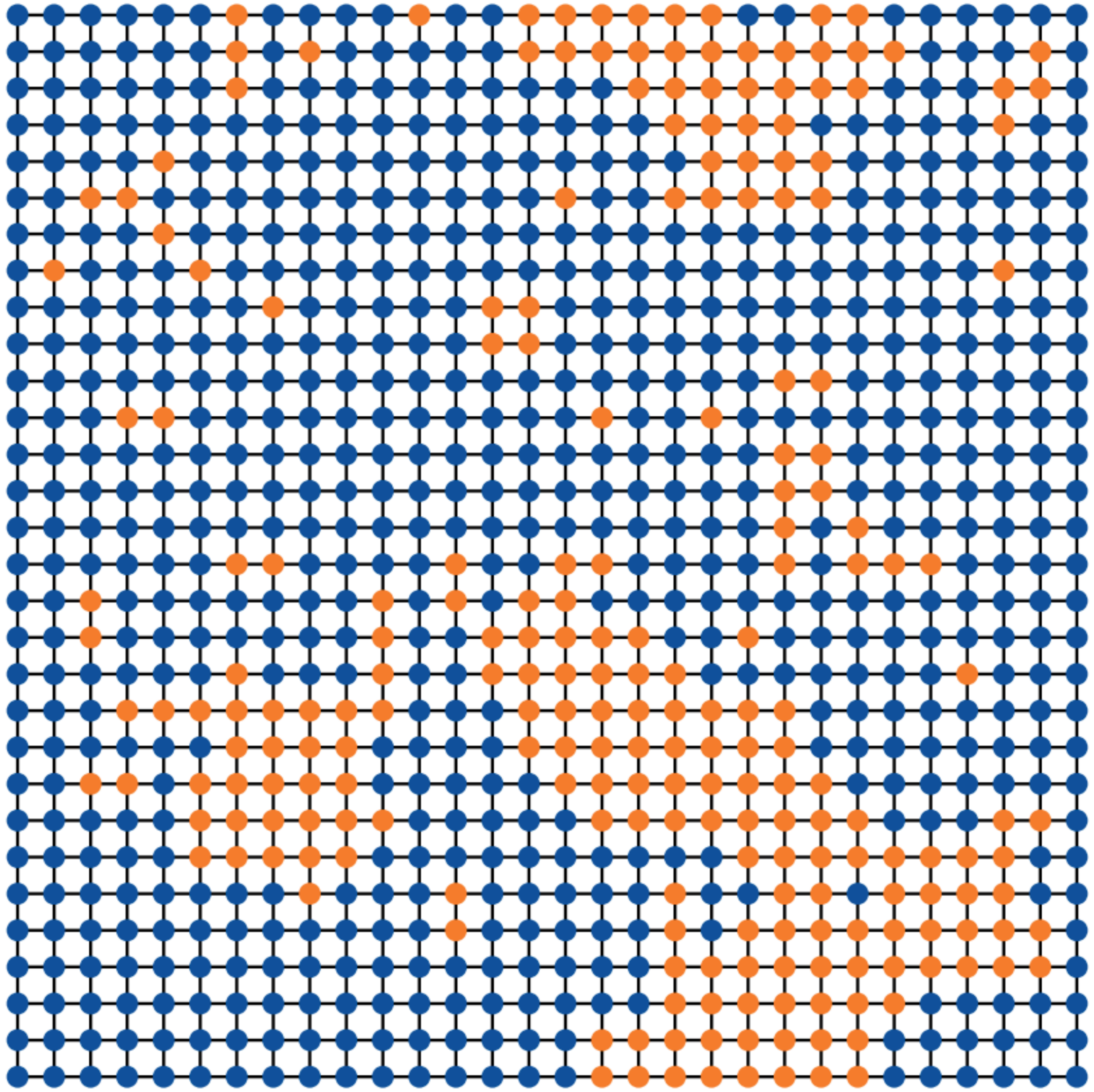


T=1.66

Simple Example: Ising Model

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j$$

temperature-driven phase transition:
ferromagnetic -> paramagnetic phase

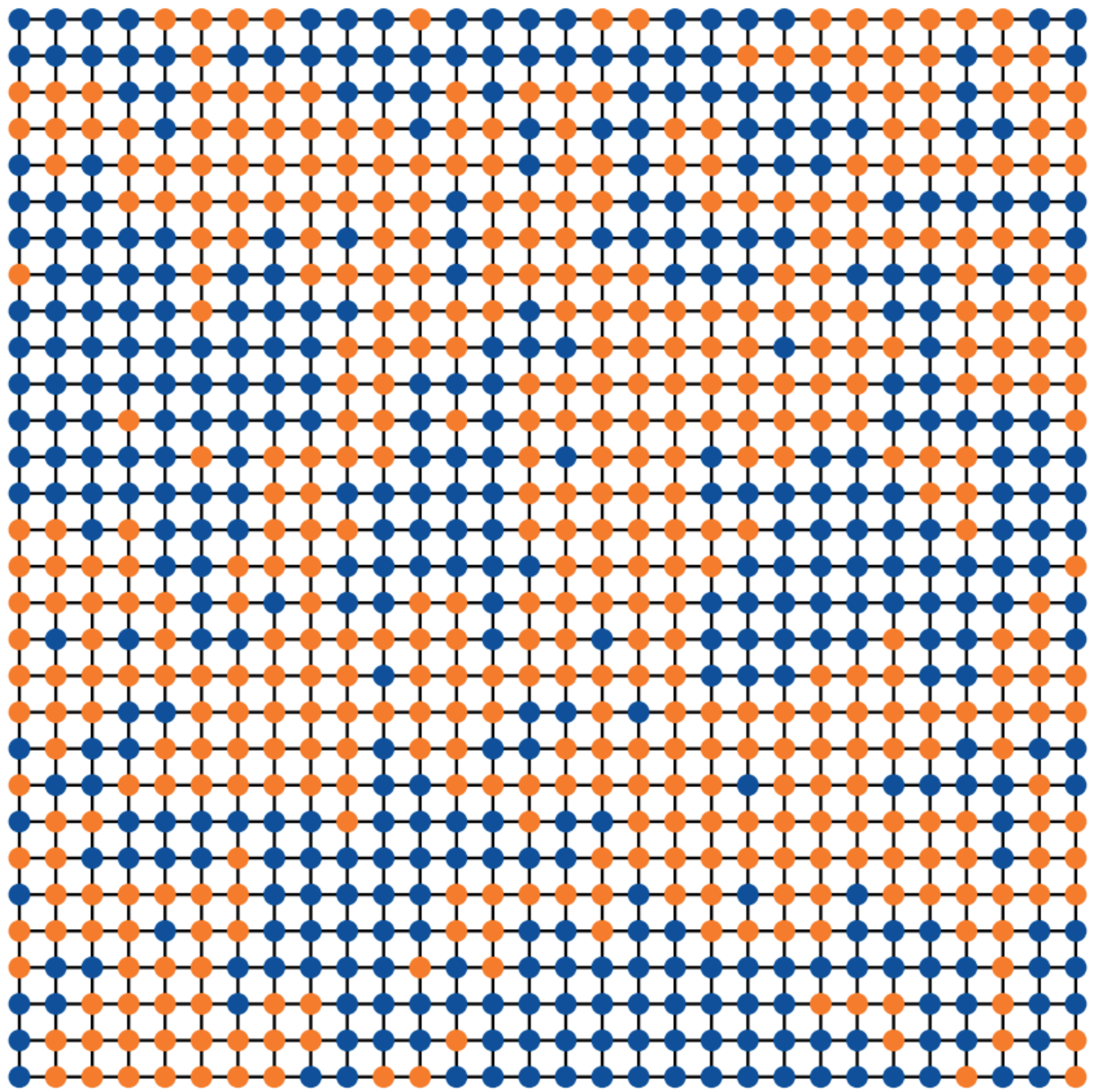


T=2.32

Simple Example: Ising Model

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j$$

temperature-driven phase transition:
ferromagnetic -> paramagnetic phase



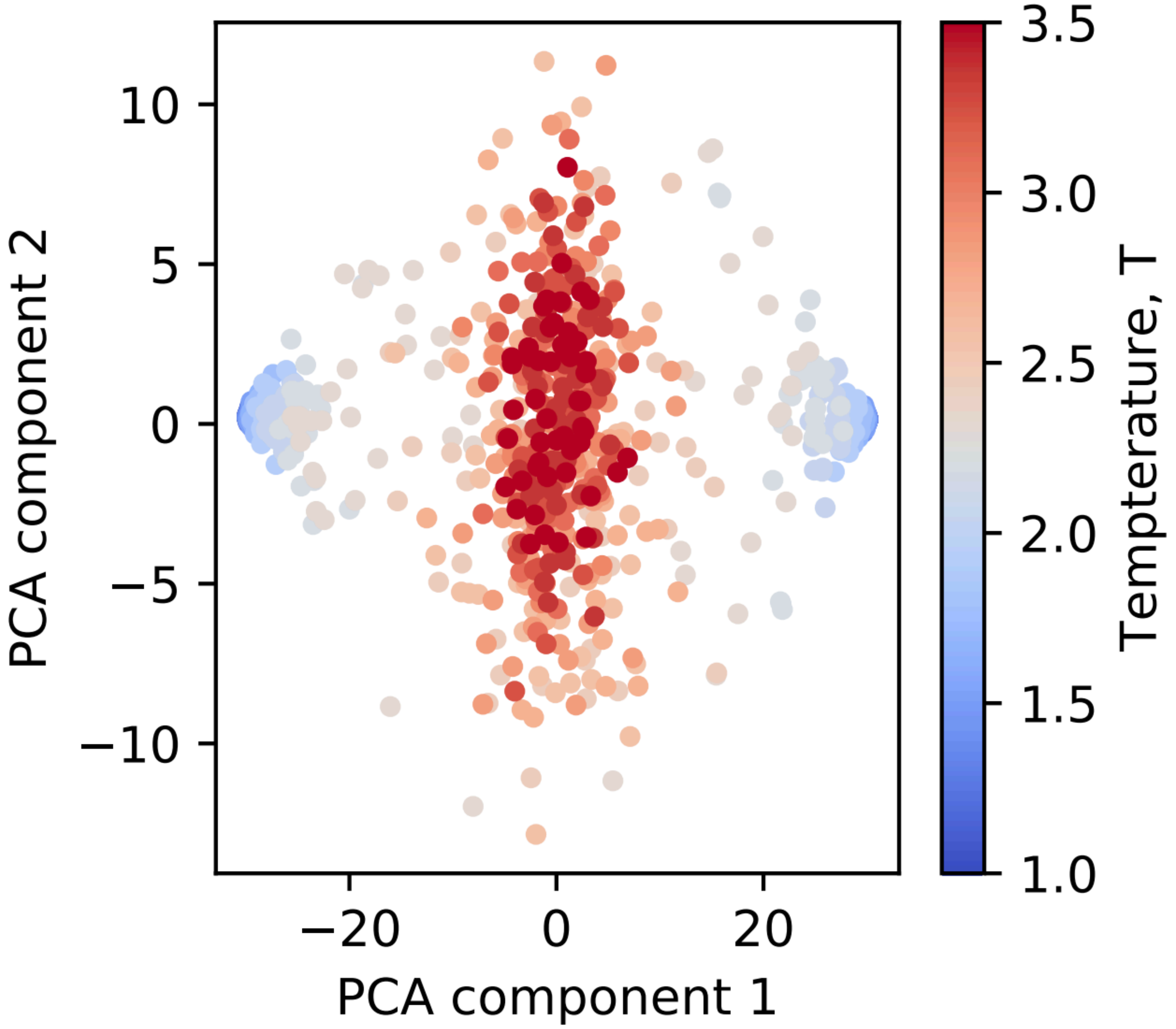
T=3.37

Simple Example: Ising Model

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j$$

temperature-driven phase transition:
ferromagnetic -> paramagnetic phase

Principal Component Analysis



Lei Wang, PHYSICAL REVIEW B 94, 195105 (2016)

Simple Example: Ising Model

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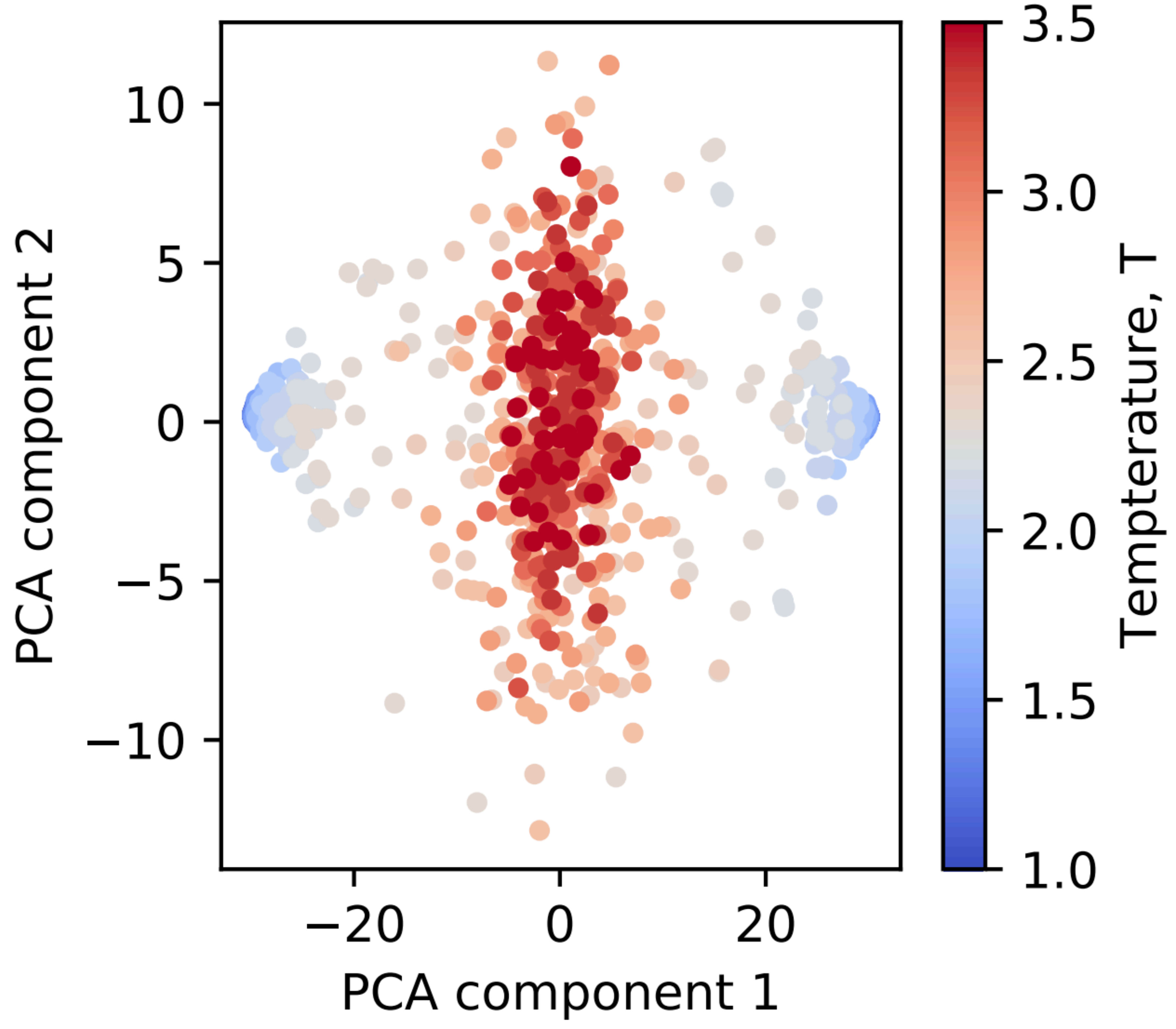
Principal Component Analysis



https://colab.research.google.com/drive/1CZCp42y07Wym73GkVQerlza7vnWd4Smd

Lei Wang, PHYSICAL REVIEW B 94, 195105 (2016)

Harder models: Confusion schemes, VAEs, RL …

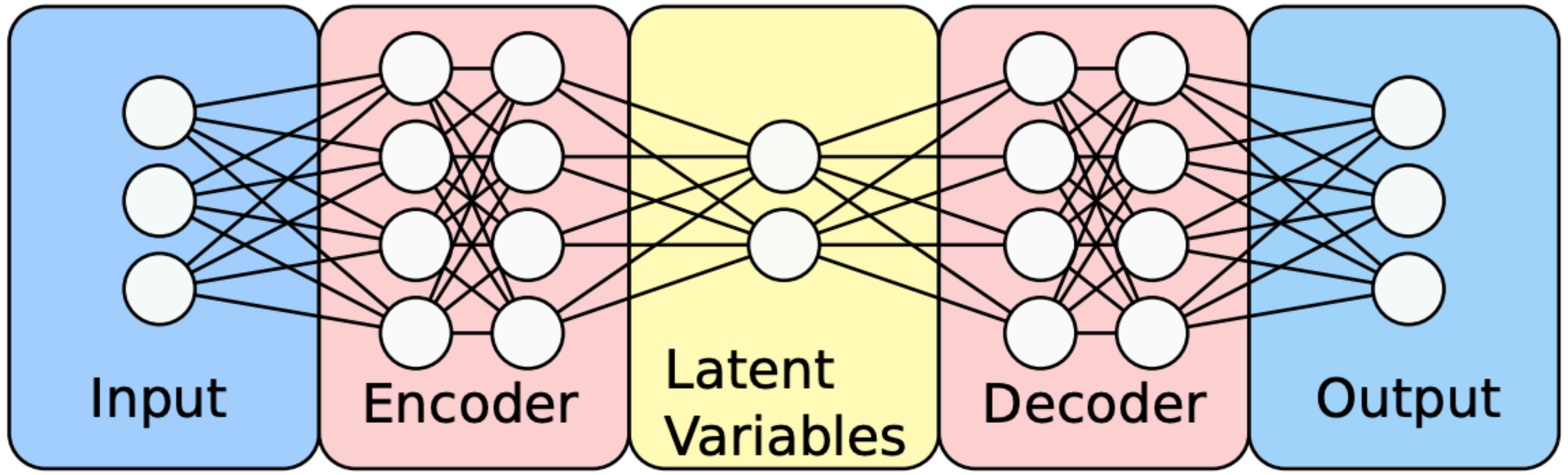
Unsupervised learning of phase transitions: From principal component analysis to variational autoencoders

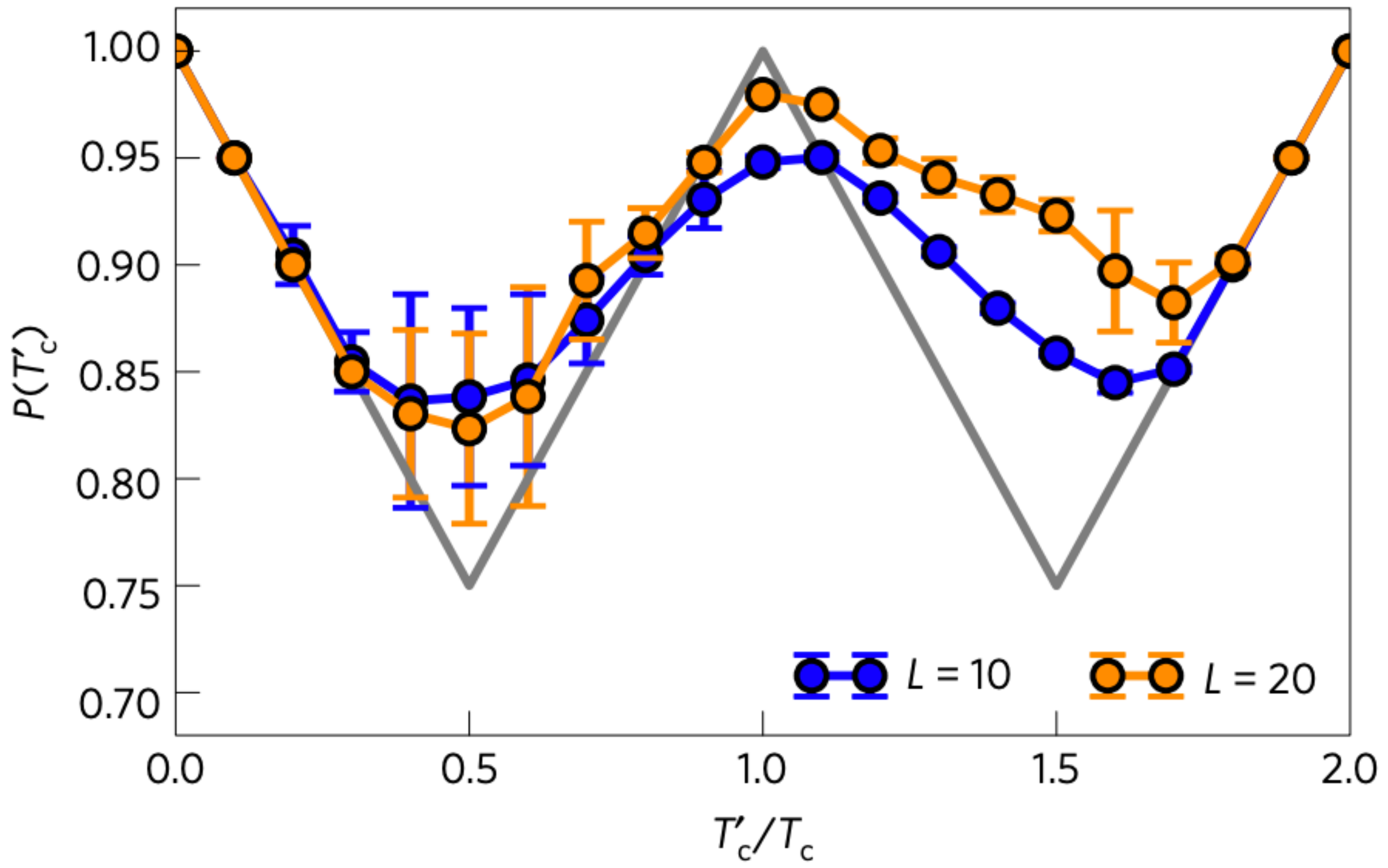
Sebastian J. Wetzel
Phys. Rev. E **96**, 022140 – Published 18 August 2017

nature physics LETTERS
PUBLISHED ONLINE: 13 FEBRUARY 2017 | DOI: 10.1038/NPHYS4037

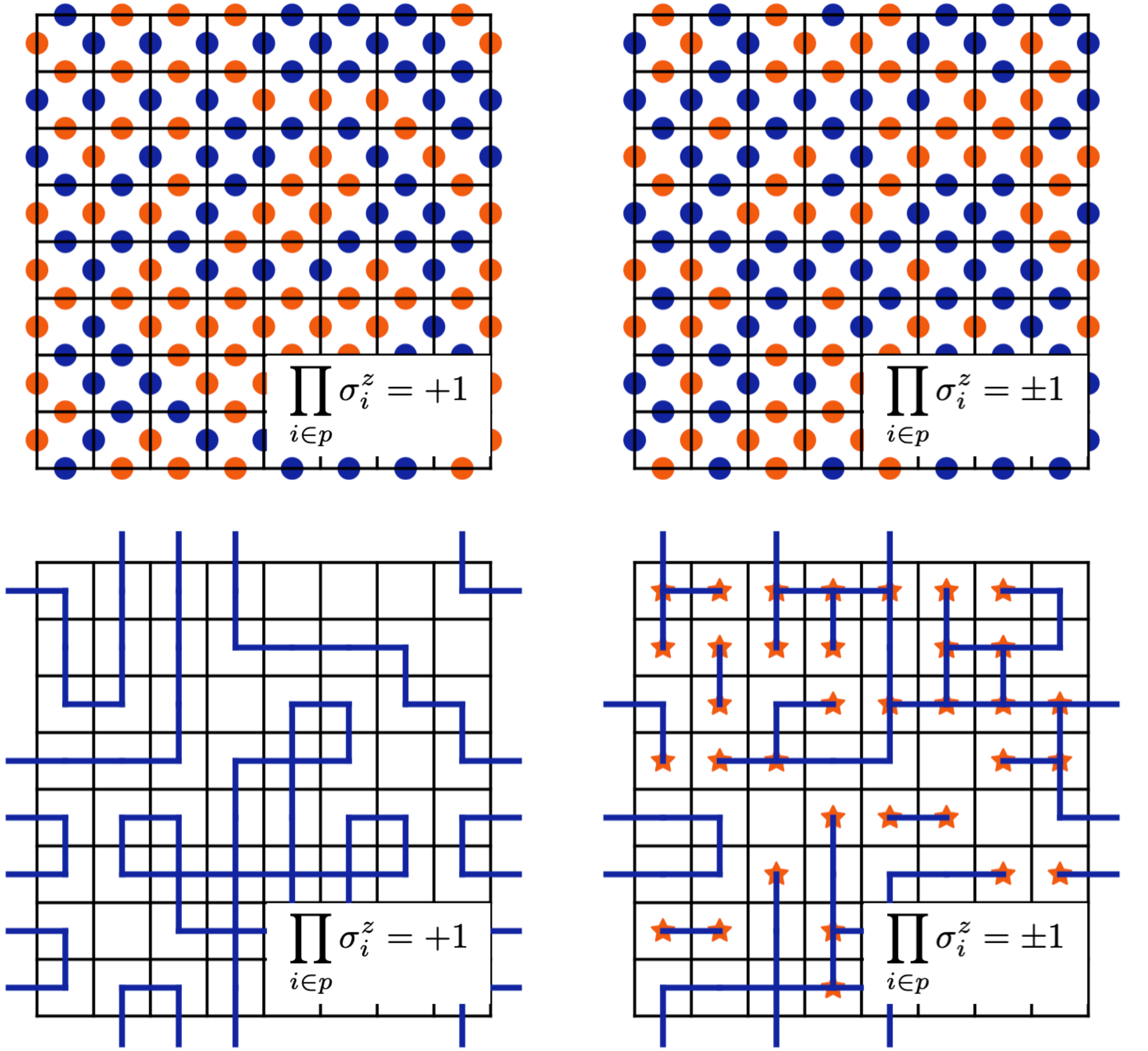
Learning phase transitions by confusion

Evert P. L. van Nieuwenburg*, Ye-Hua Liu and Sebastian D. Huber

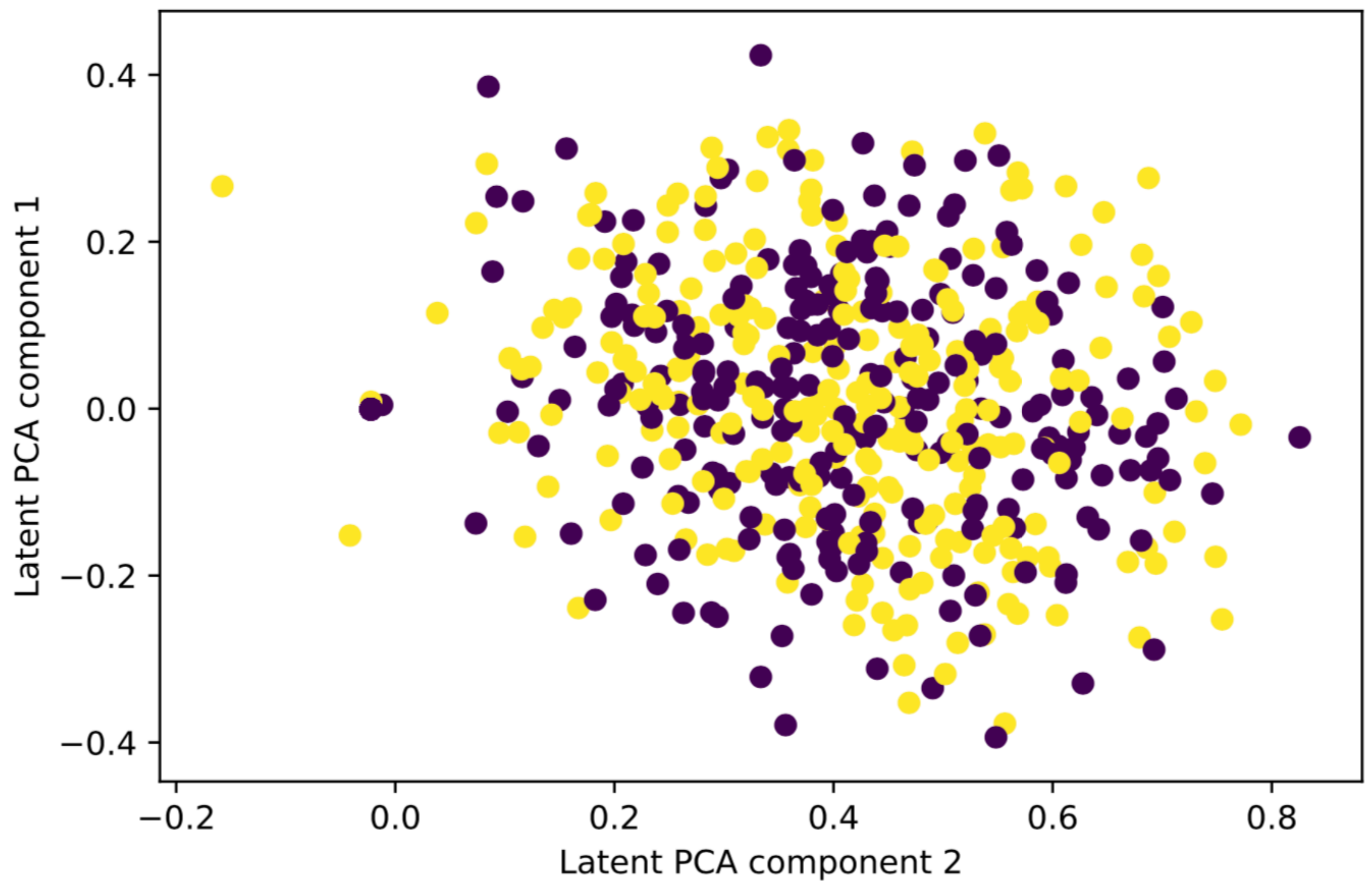




Tricky example: Ising Gauge Theory



$$H_{IGT} = -J\sum_{p}\prod_{i\in p}\sigma_i^z$$

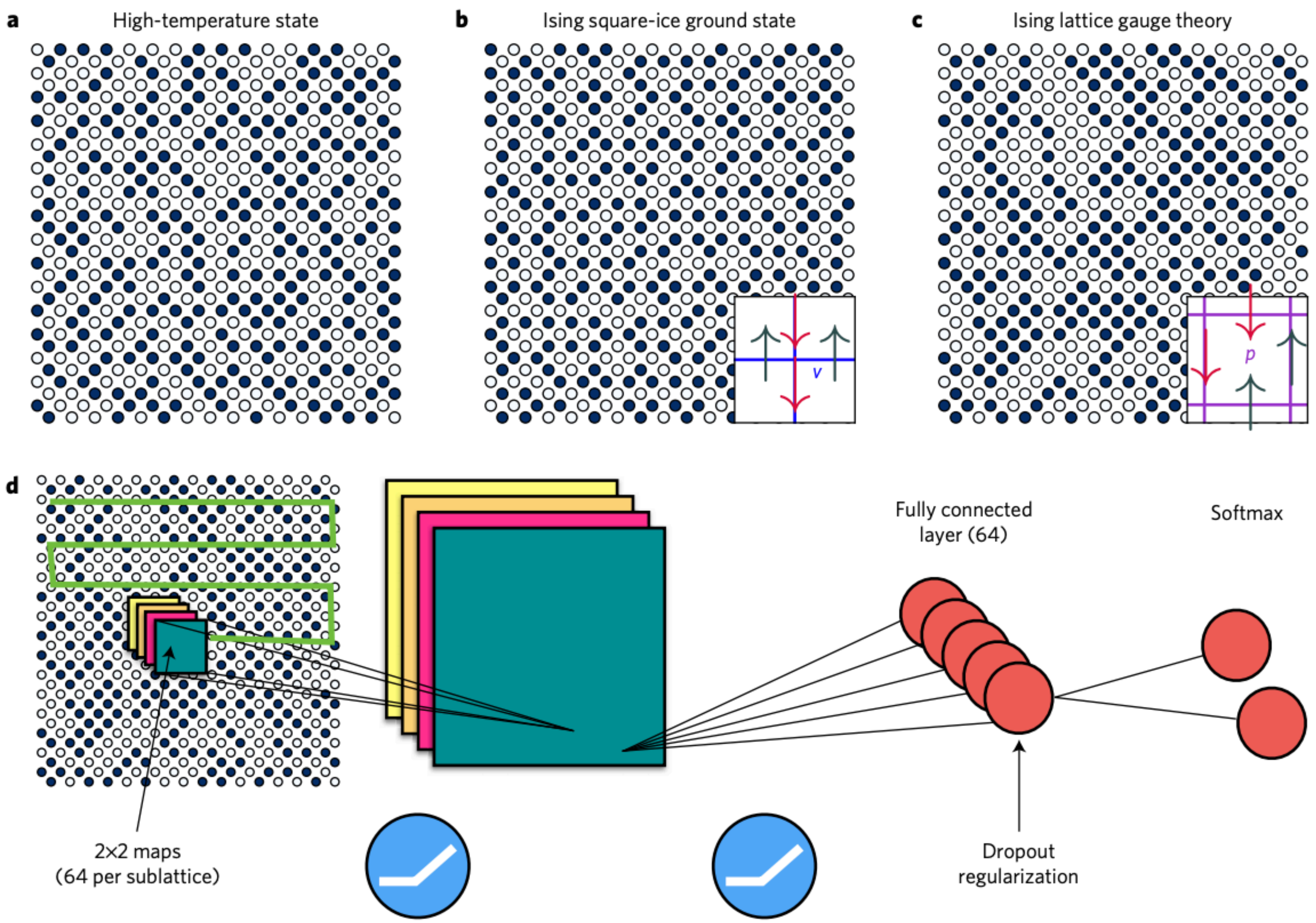


Supervised learning

nature physics
LETTERS
PUBLISHED ONLINE: 13 FEBRUARY 2017 | DOI: 10.1038/NPHYS4035

Machine learning phases of matter

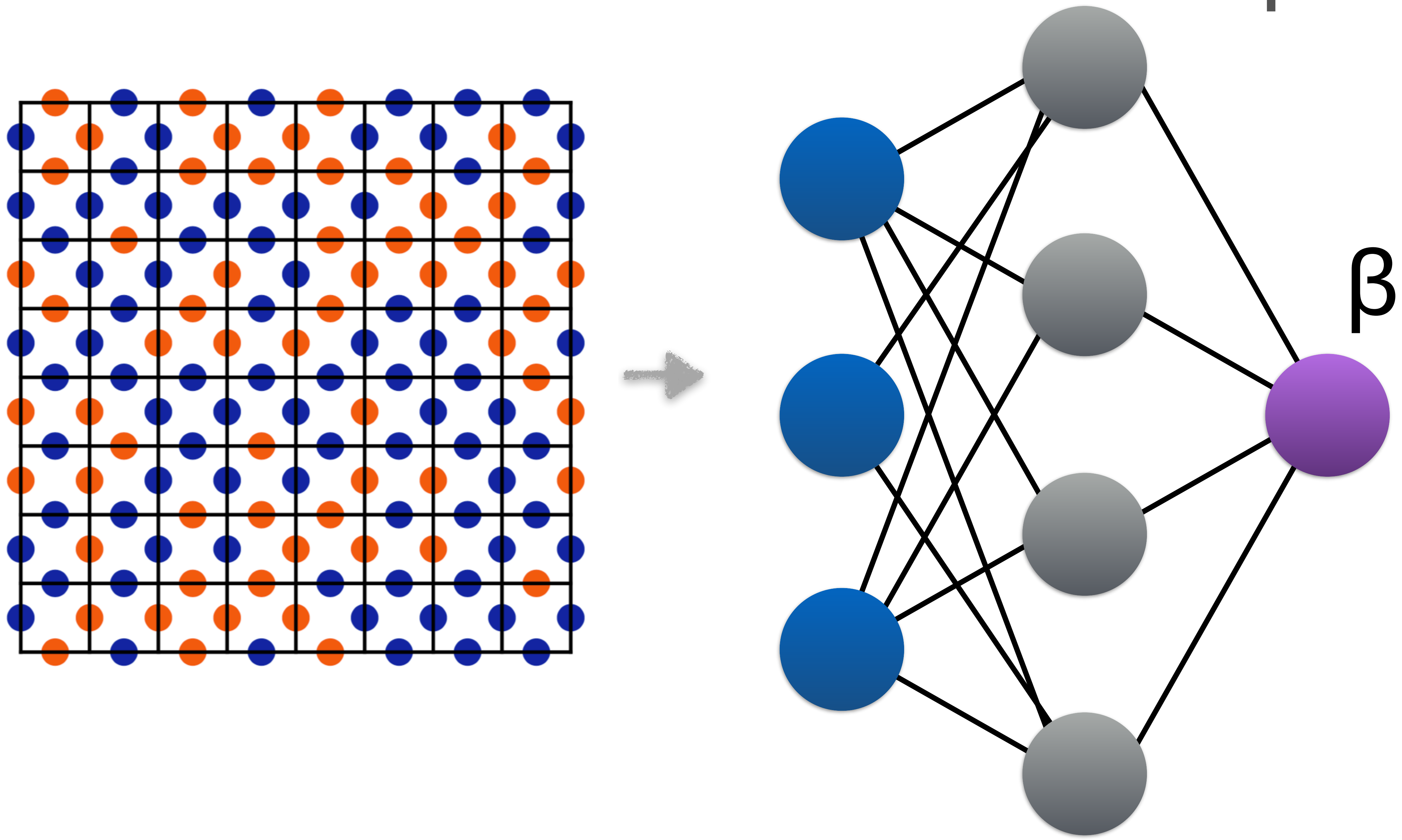
Juan Carrasquilla[1*] and Roger G. Melko[1,2]



Our method

Train on configurational data

Learn to predict inverse temperature



1. Pick continuous parameter(s) of the system
2. Pick an observable of the system
3. Train a neural network to predict parameters given observables
4. Apply the model on a set of new data
5. Around a phase transition the network predictions will diverge

EG, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, S. Huber, arXiv: 1910.10124
F. Schäfer, N. Lörch, Phys. Rev. E 99, 062107 (2019)

Our method

1. Pick continuous parameter(s) of the system

Inverse temperature:

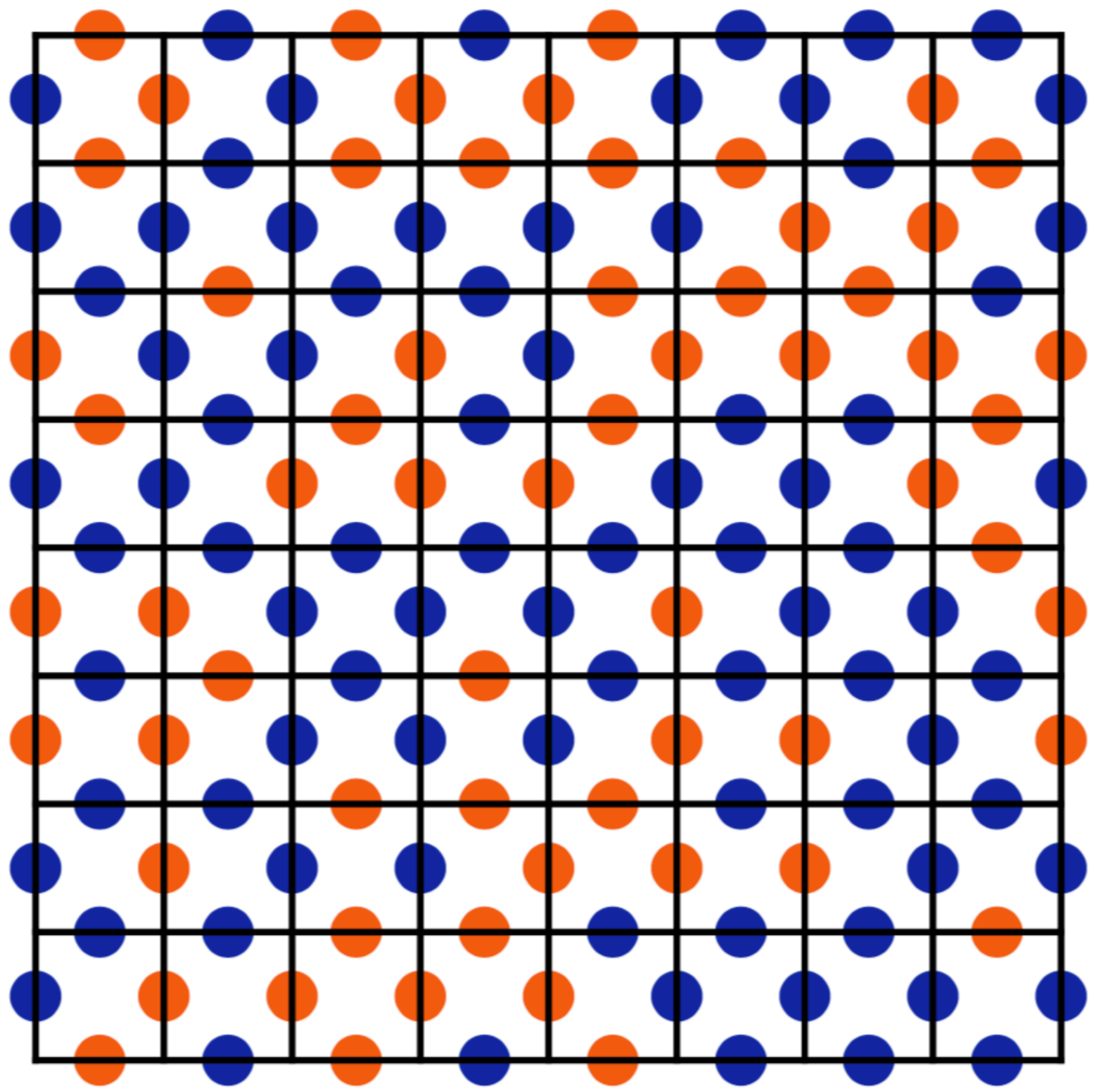
$$\beta = \frac{1}{T}$$

EG, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, S. Huber, arXiv: 1910.10124

Our method

2. Pick an observable of the system

Configuration:



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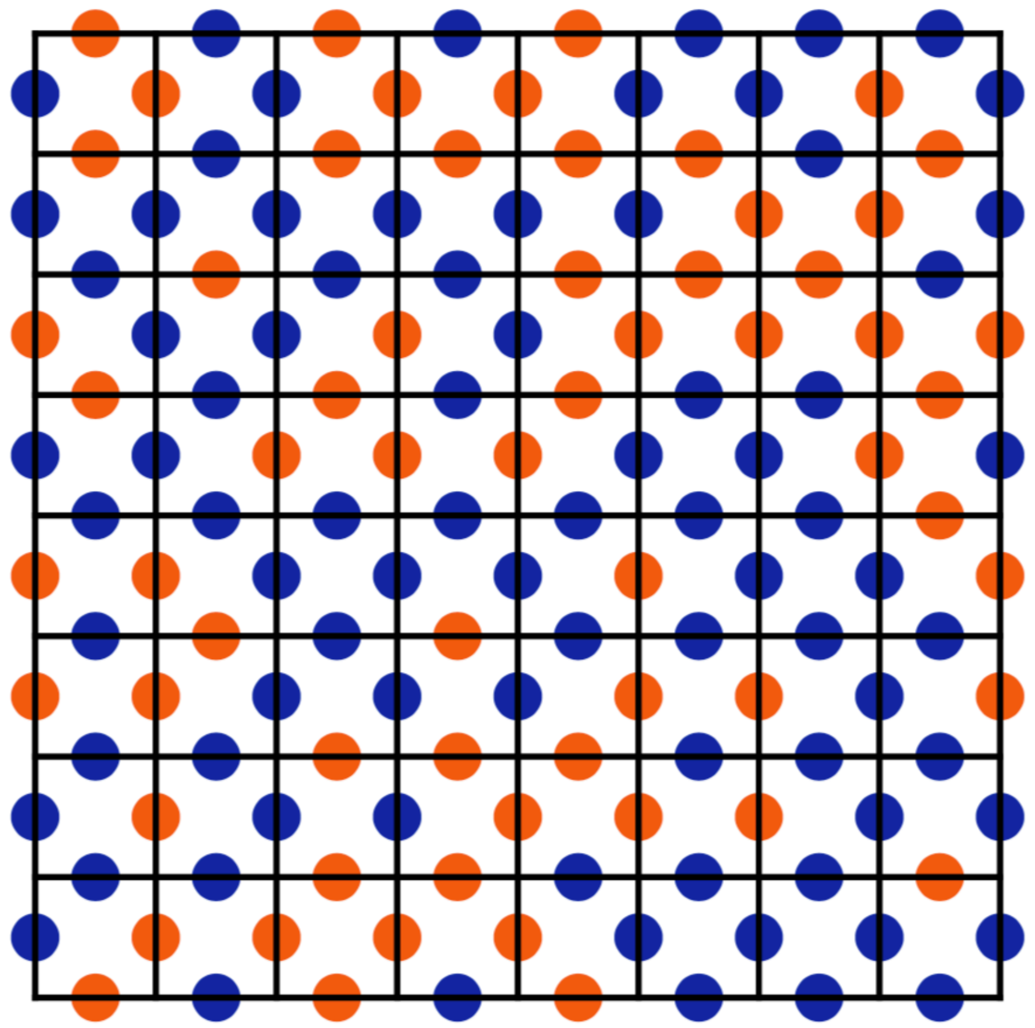
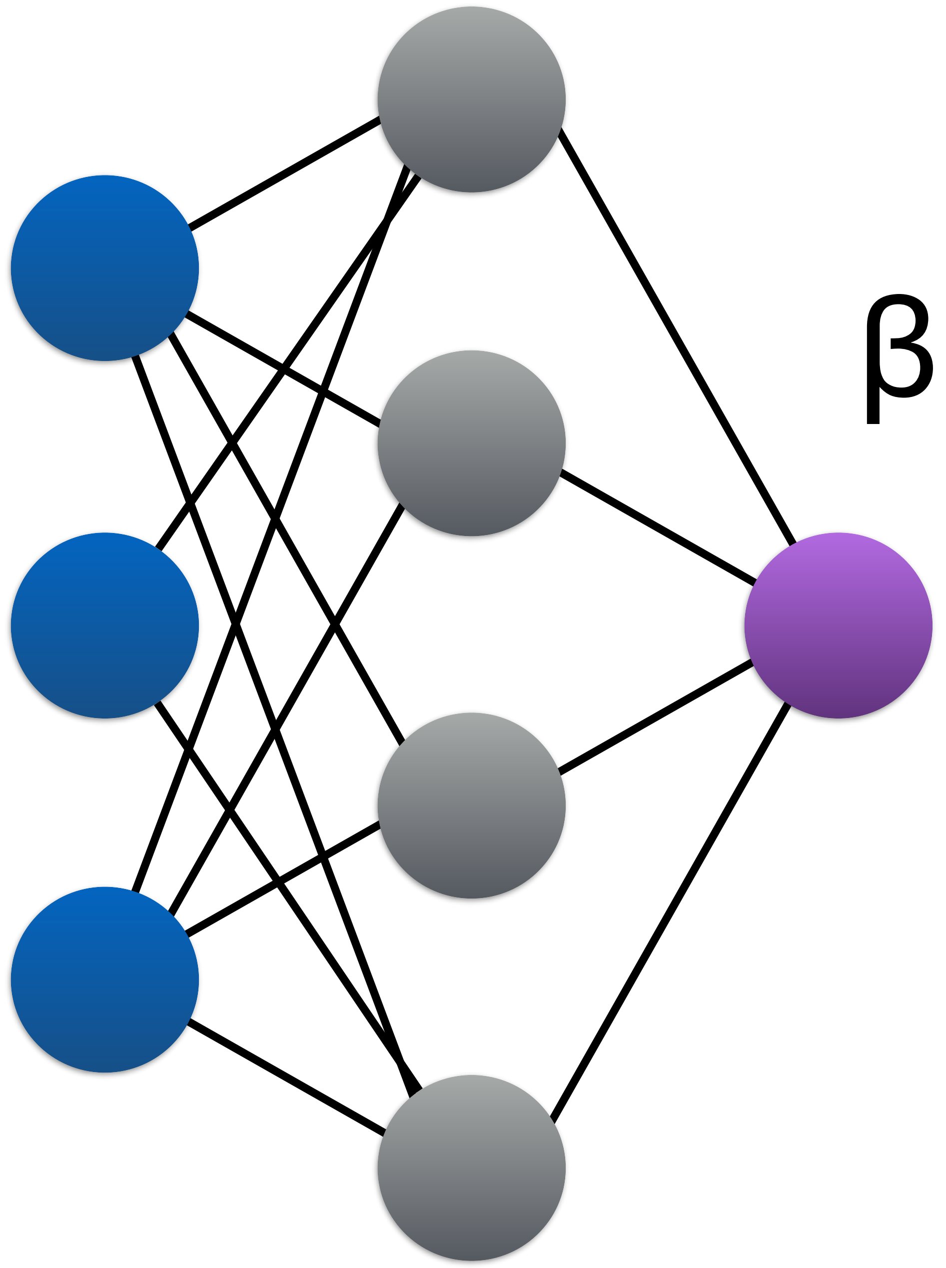
Our method

3. Train a neural network to predict parameters given observables

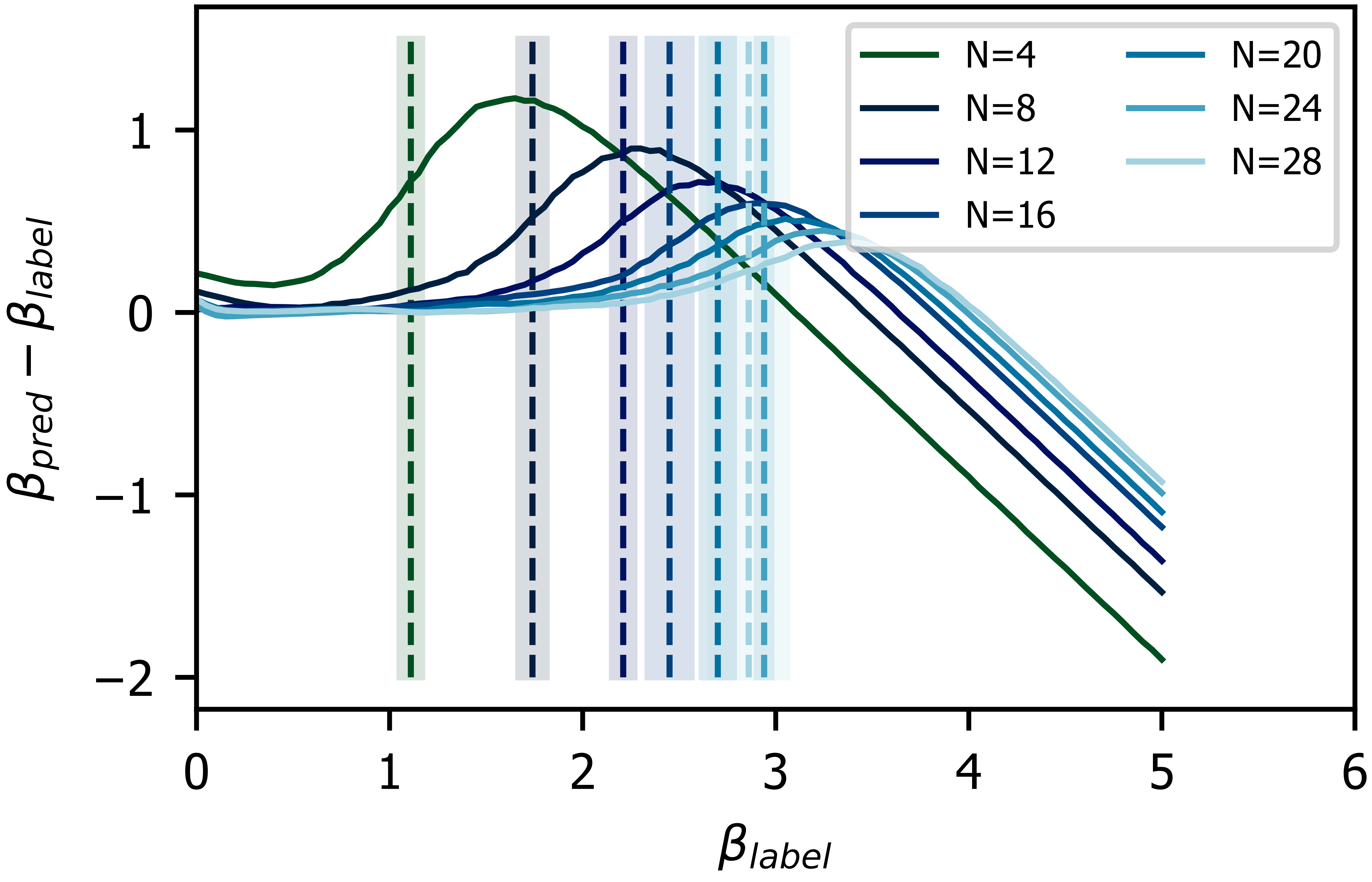




EG, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, S. Huber, arXiv: 1910.10124

Our method

4. Apply model on a new data

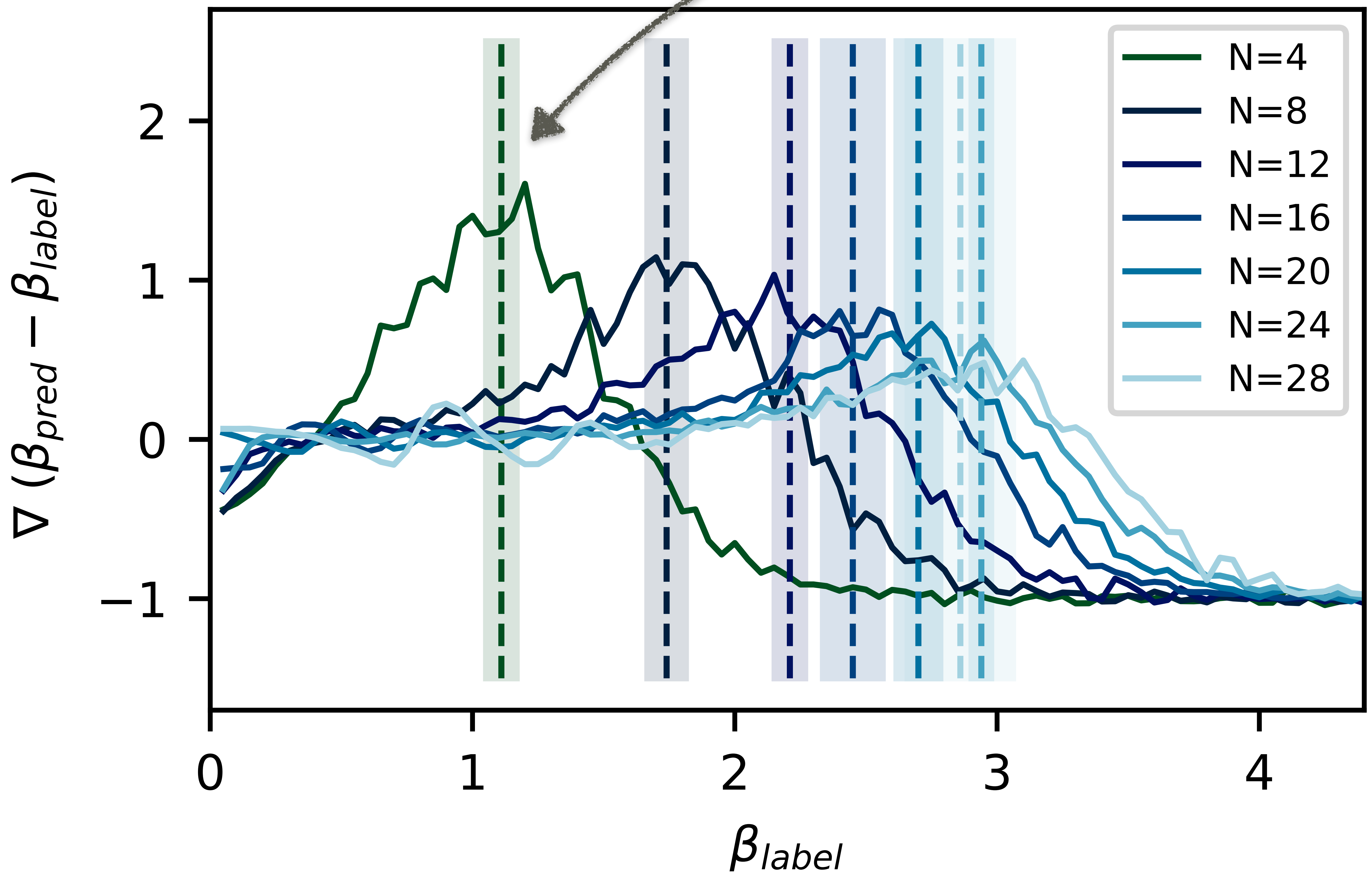


EG, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, S. Huber, arXiv: 1910.10124

Our method

The peak coincides with the position of the crossover temperature!

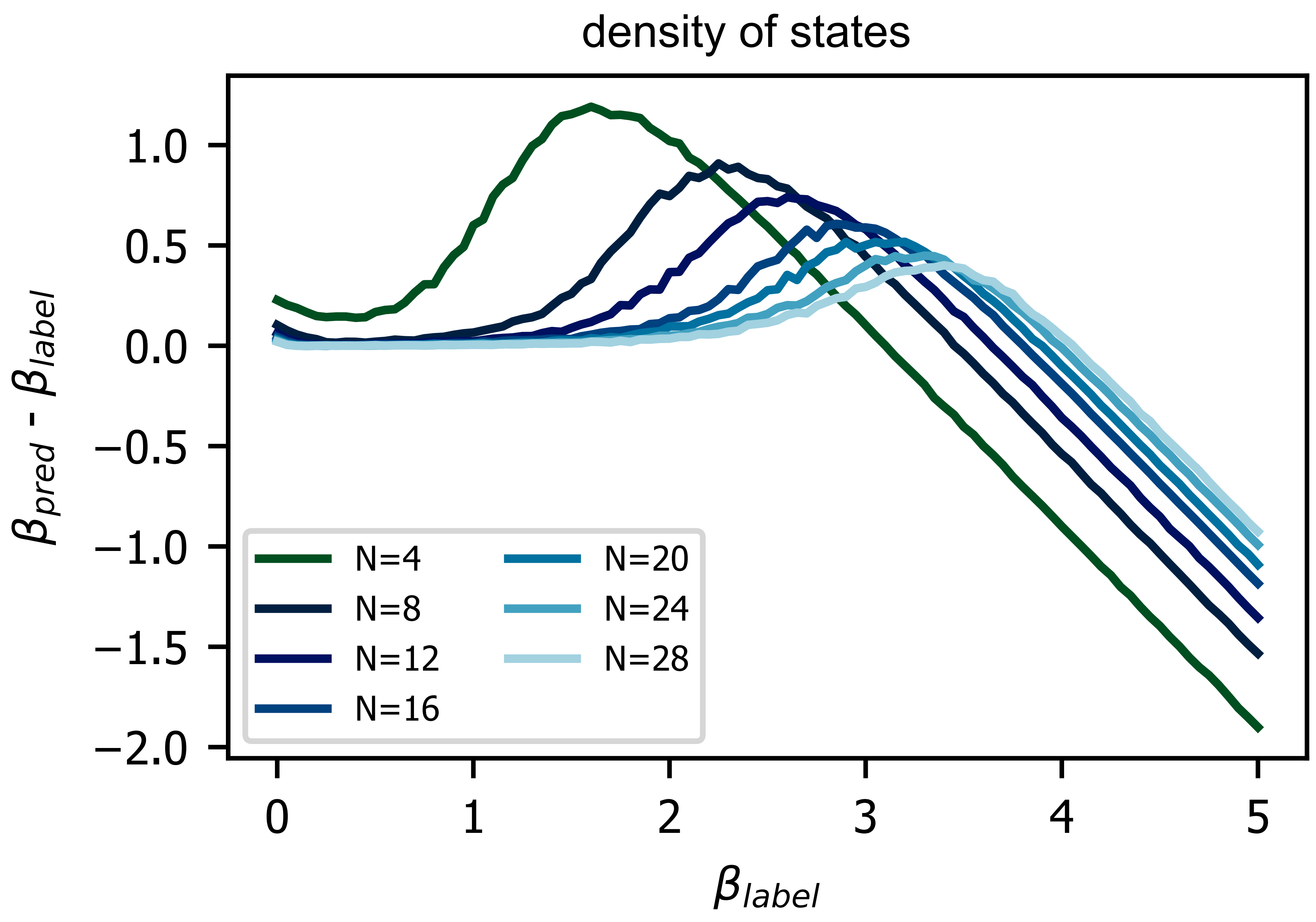
5. Look at derivative of the predictions

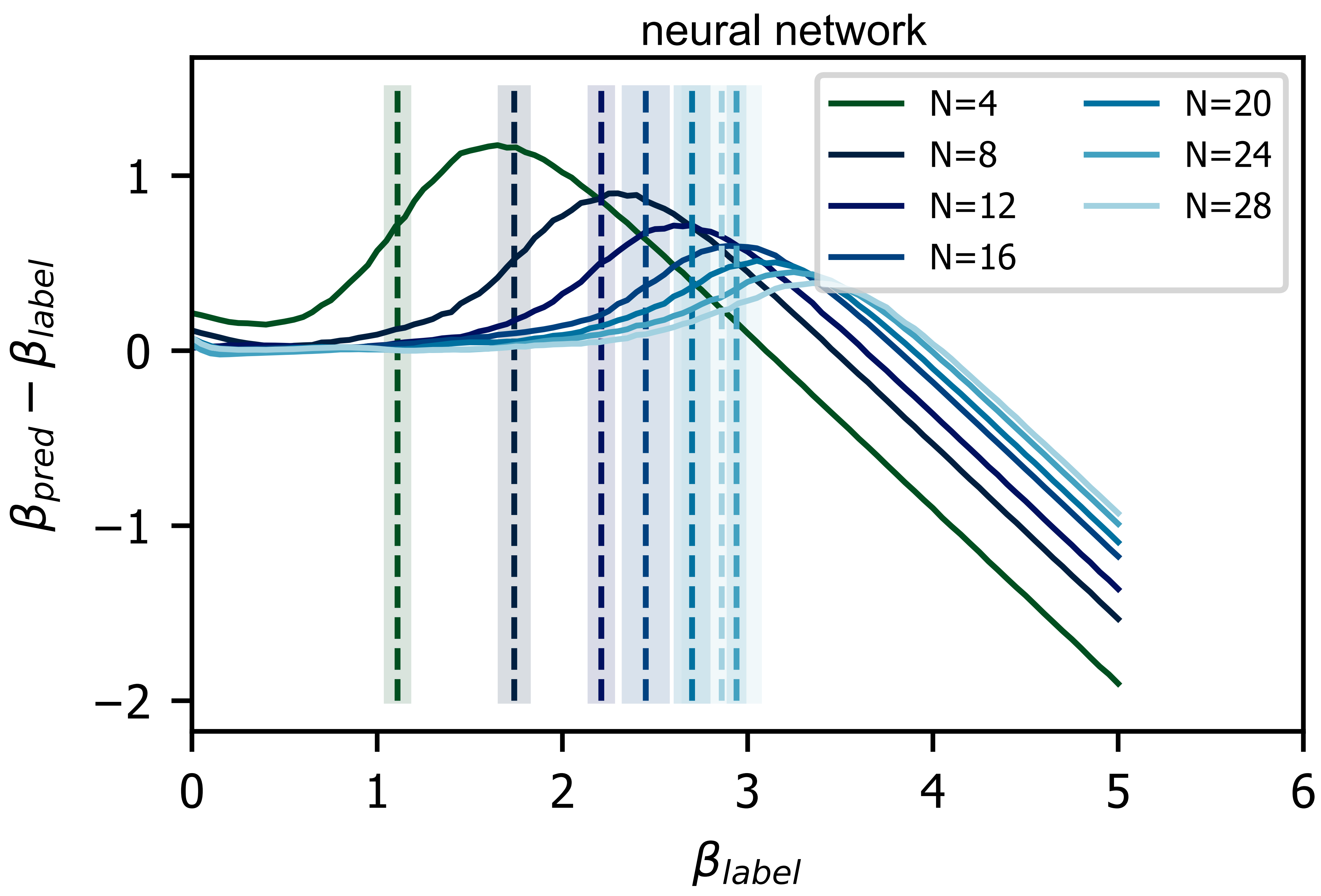


EG, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, S. Huber, arXiv: 1910.10124

Our method

6. The network is learning the density of states in the provided set of configurations!

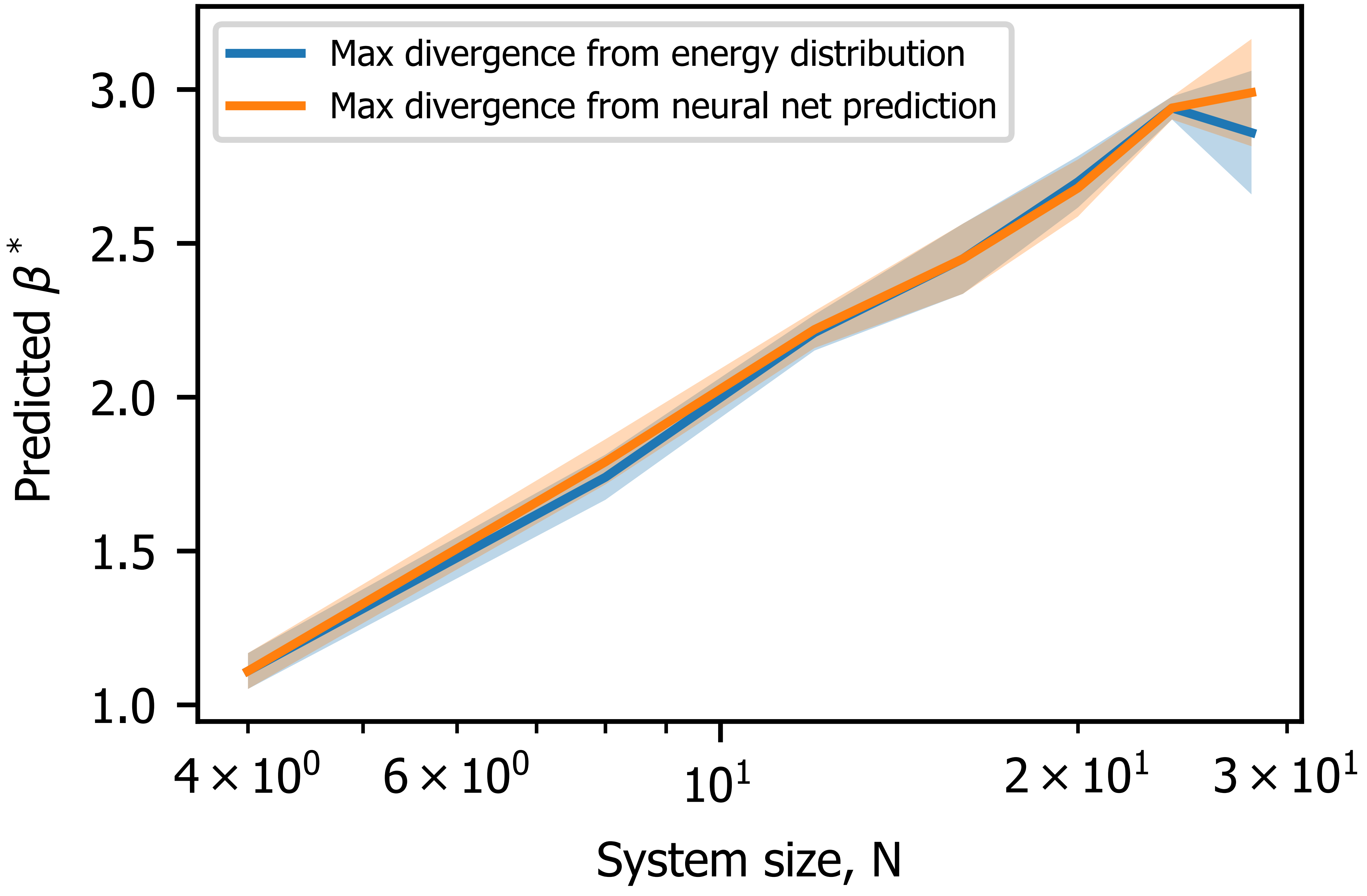


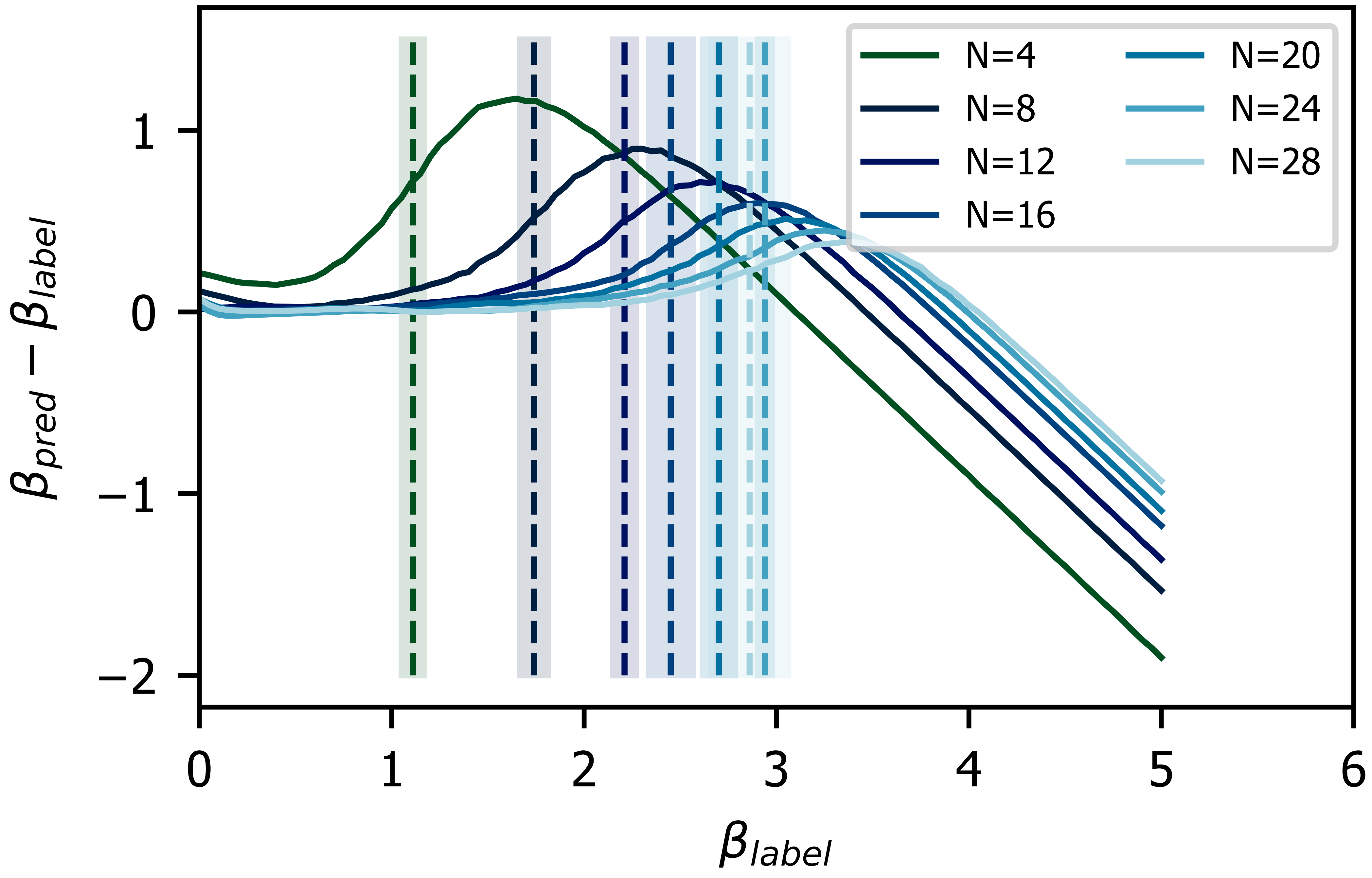


EG, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, S. Huber, arXiv: 1910.10124

Our method

Logarithmic scaling with the system size.





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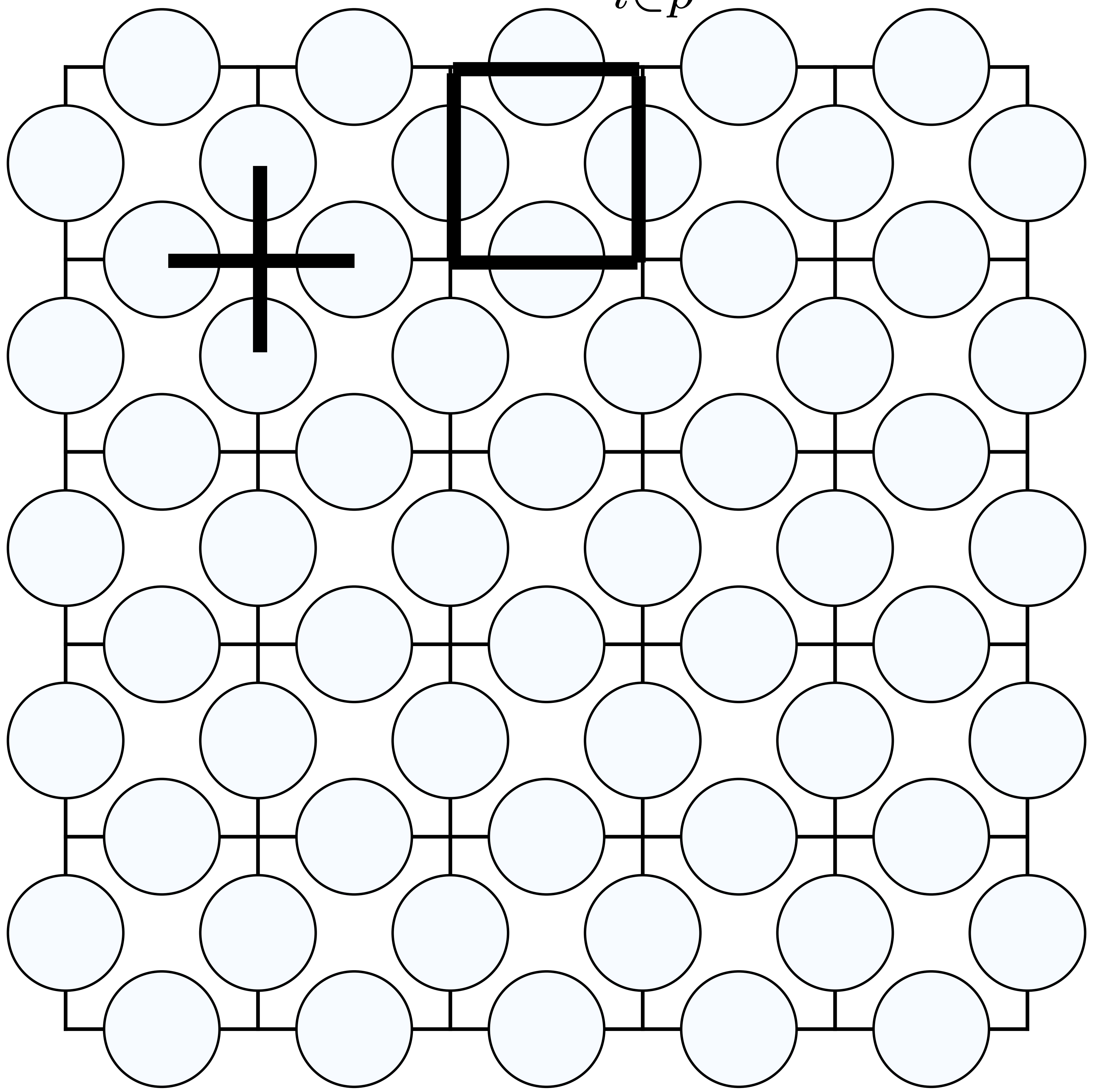
Does this work in quantum setting?

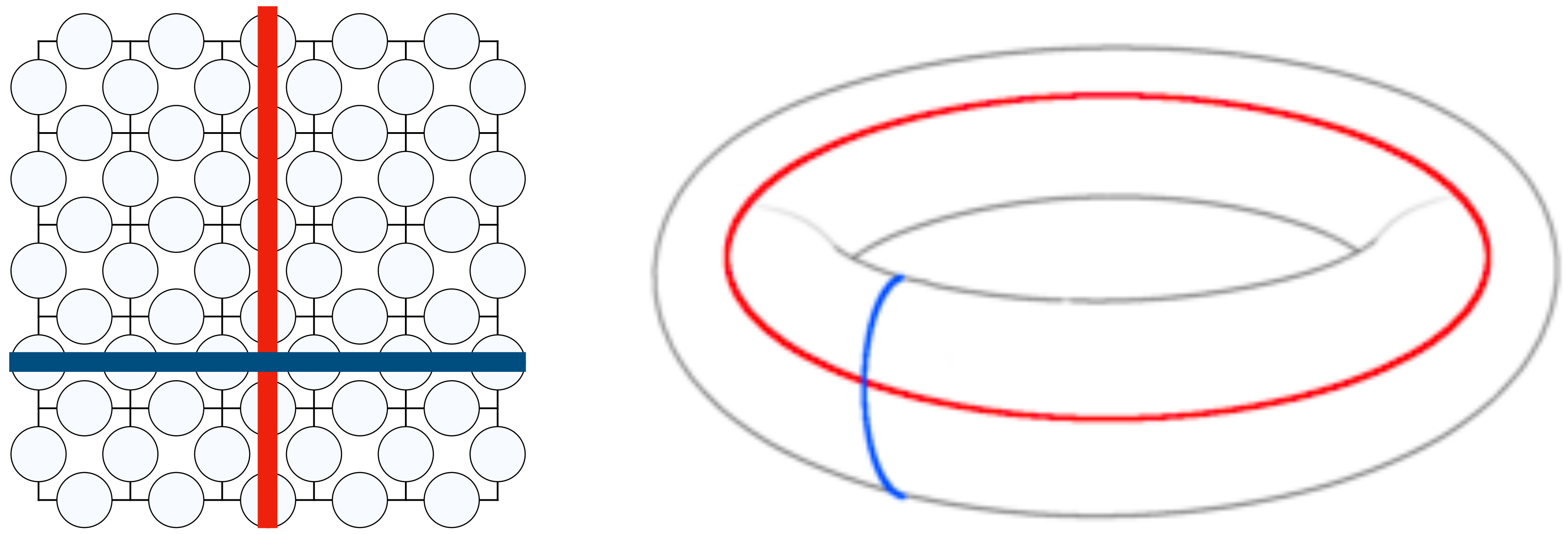
Yes!

$$H = -\sum_s A_s - \sum_p B_p$$

$$B_p = \prod_{i \in p} \sigma_i^z$$

$$A_s = \prod_{i \in s} \sigma_i^x$$



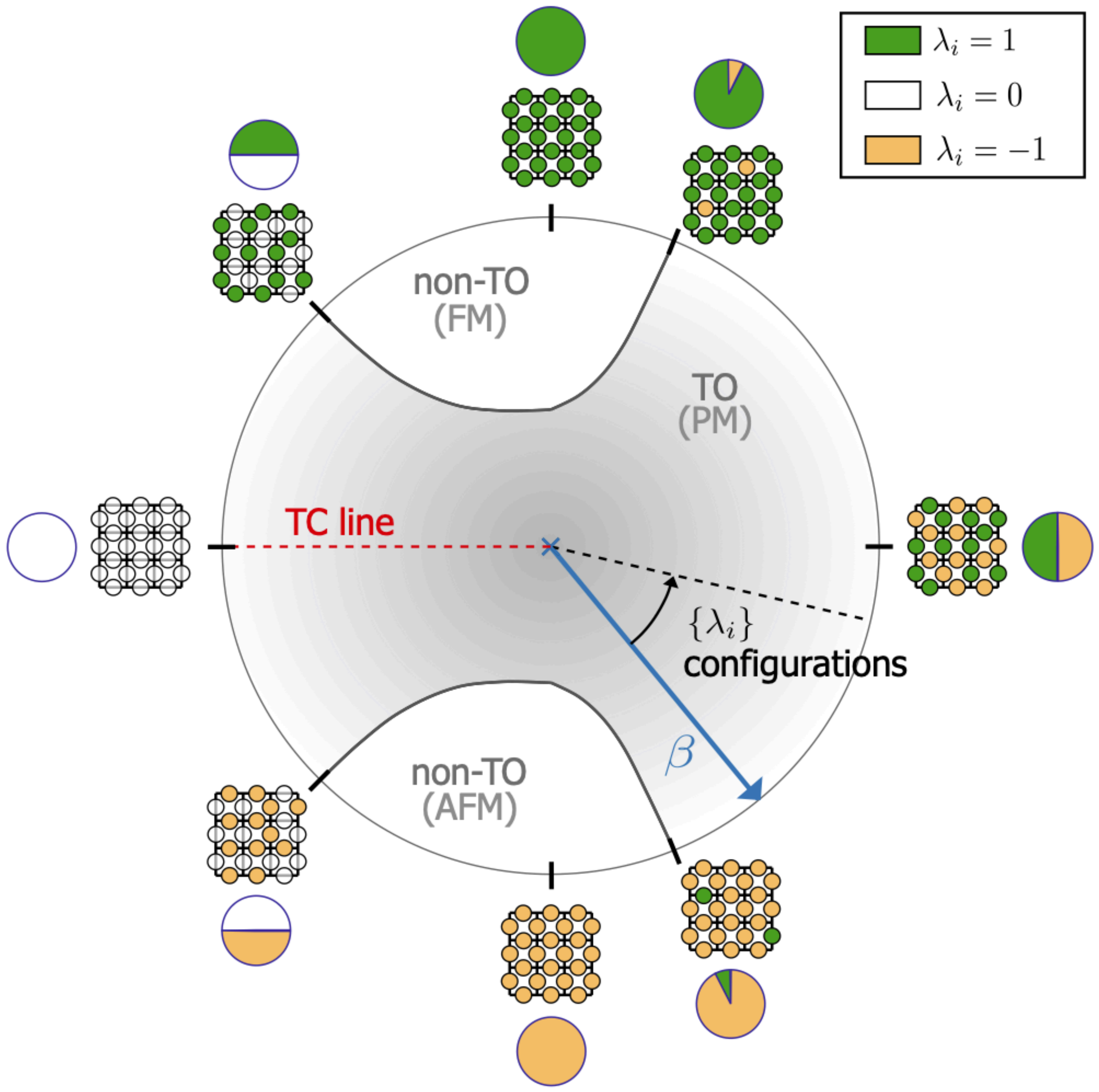


EG, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, S. Huber, arXiv: 1910.10124

A. Valenti, E. van Nieuwenburg, S. Huber, EG, PRResearch 1, 033092 (2019)

Relevant Problem: Quantum Model with Topological Phase Transition

$$H = \sum_s \left(-A_s + e^{-\sum_{i\in s} \beta_{z,i}\sigma_i^z} \right) - \sum_p B_p$$



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A. Valenti, E. van Nieuwenburg, S. Huber, EG, PRResearch 1, 033092 (2019)

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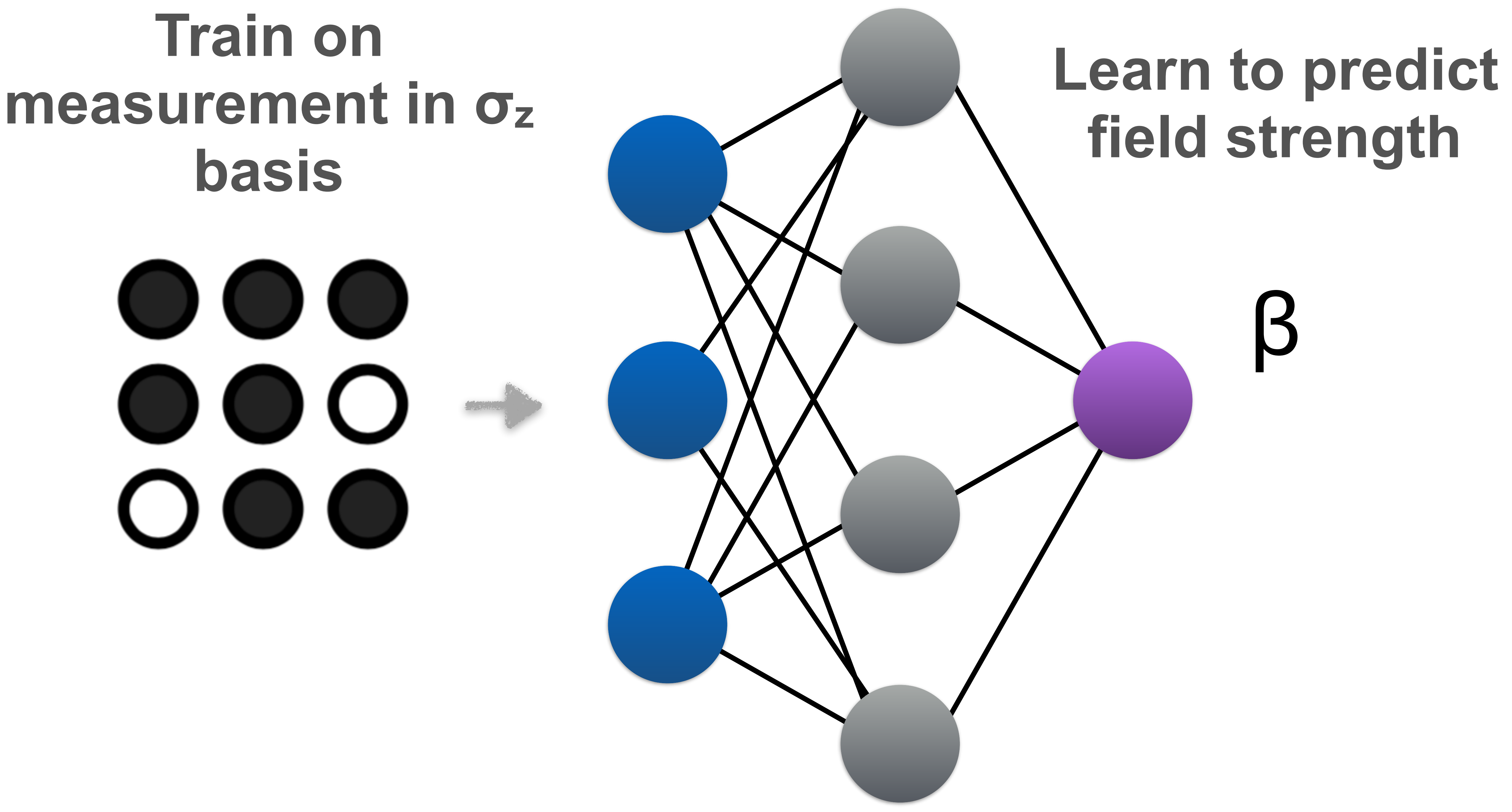

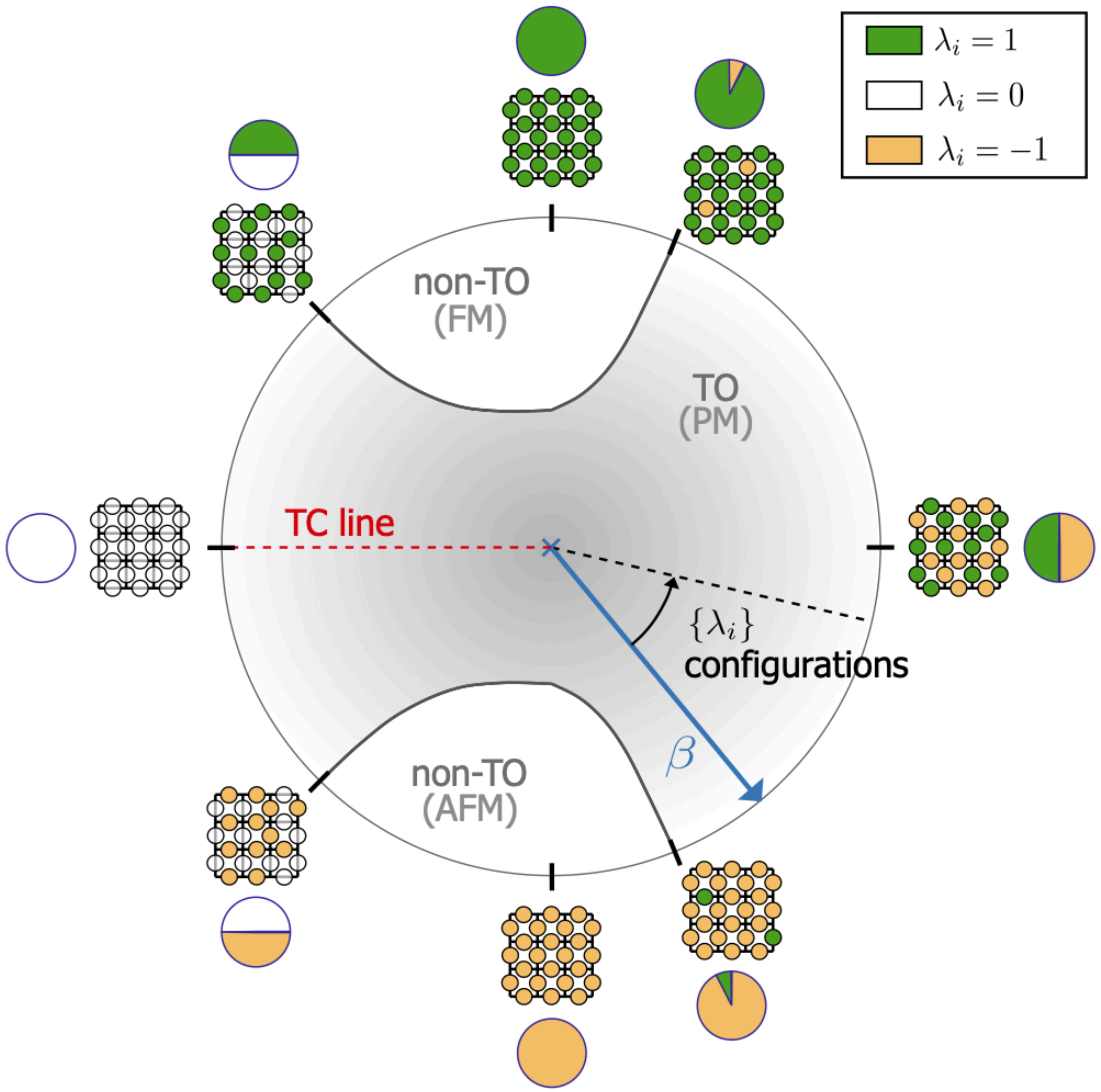

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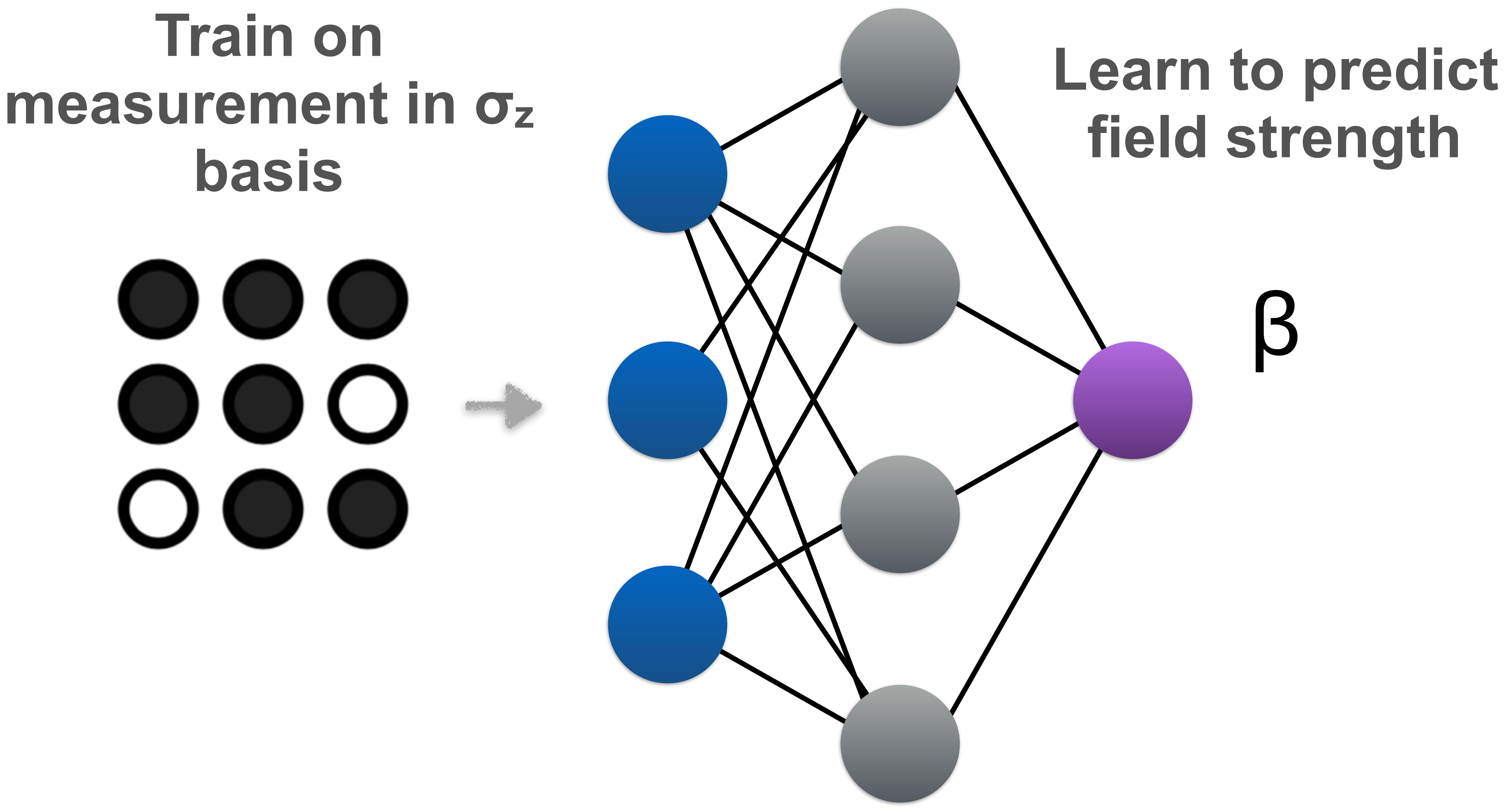

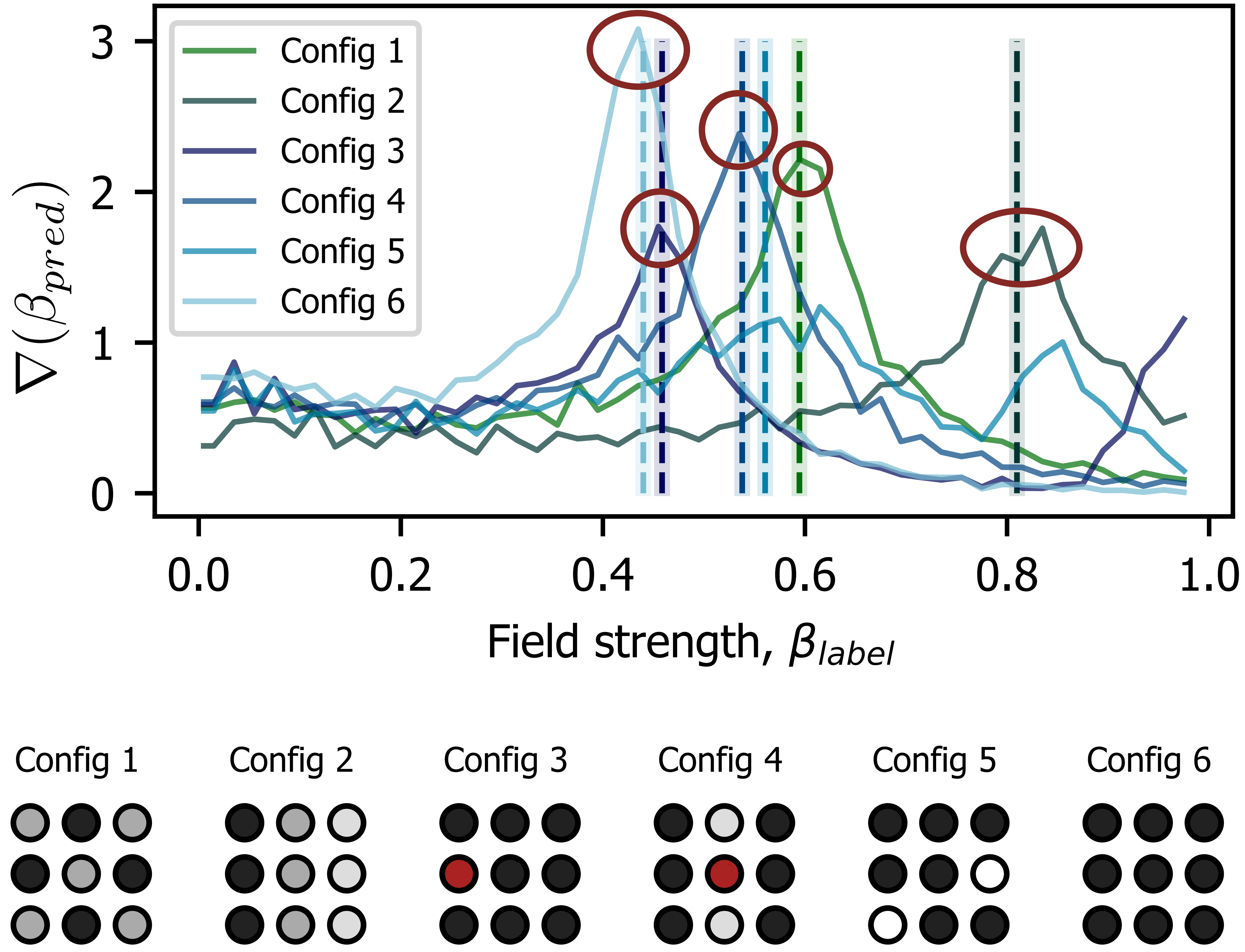

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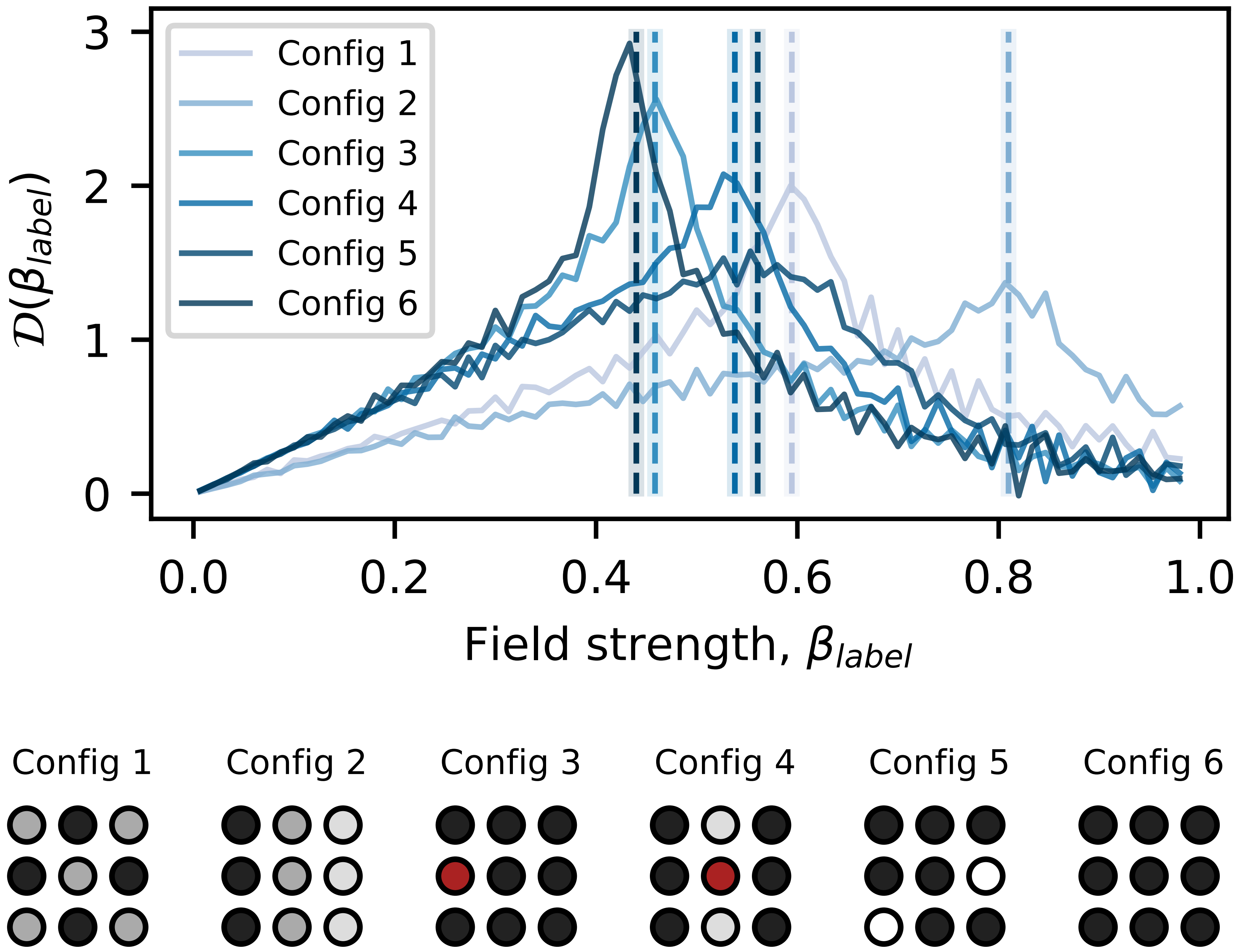
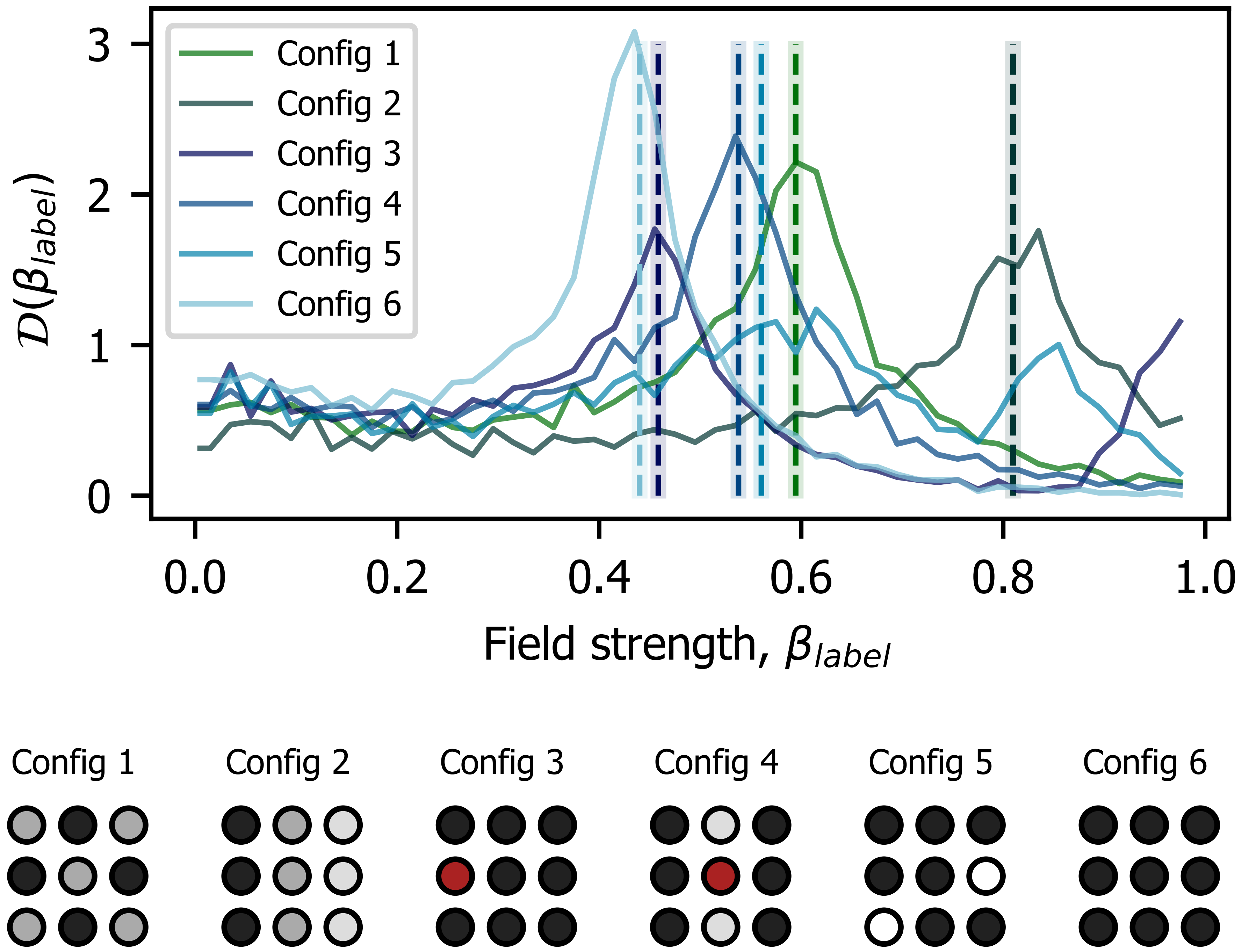
Type of measurement does not matter

$\langle A_s \rangle$



$\sigma_z - projections$



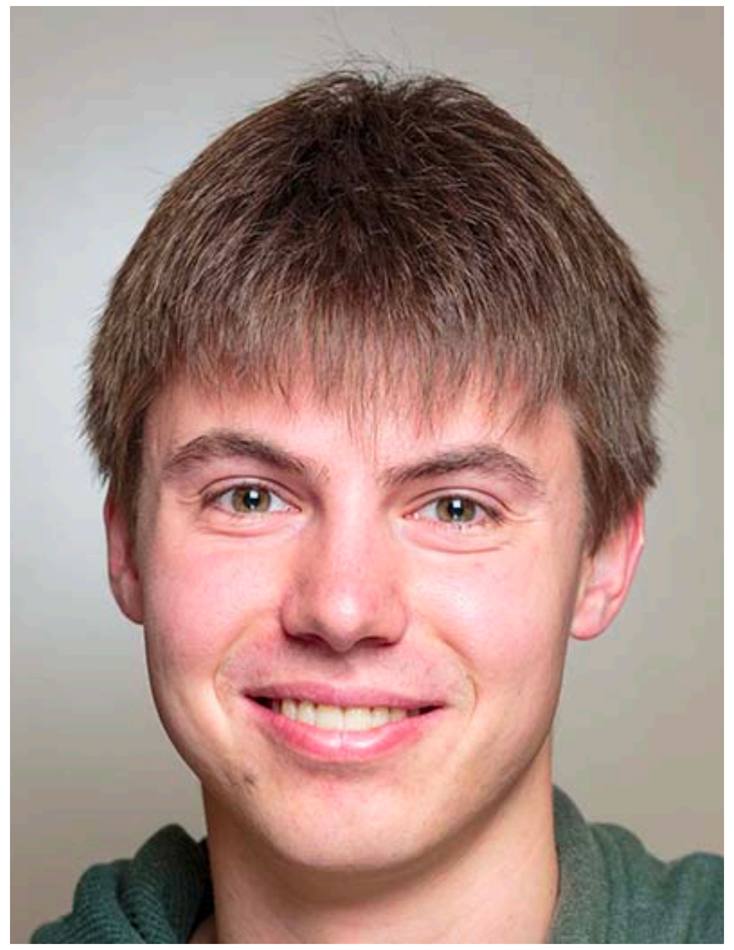
EG, A. Valenti, G. Boschung, F. Schäfer, N. Lörch, S. Huber, arXiv: 1910.10124

“Unsupervised way to determine phase boundaries (even the difficult ones!) from experimentally accessible data.”

Agnes Valenti
ETHZ

Evert van Nieuwenburg
Niels Bohr Institute

Sebastian Huber
ETHZ



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Niels Lörch
Uni Basel

Frank Schäfer
Uni Basel

arXiv: 1910.10124
arXiv: 1907.02540 (PRResearch 1, 033092(2019))
GIT: cmt-qo/cm-phaseTransitions, cmt-qo/cm-toricCode

@EliskaGreplova @Evert_vN @CmtQo @hubersebi