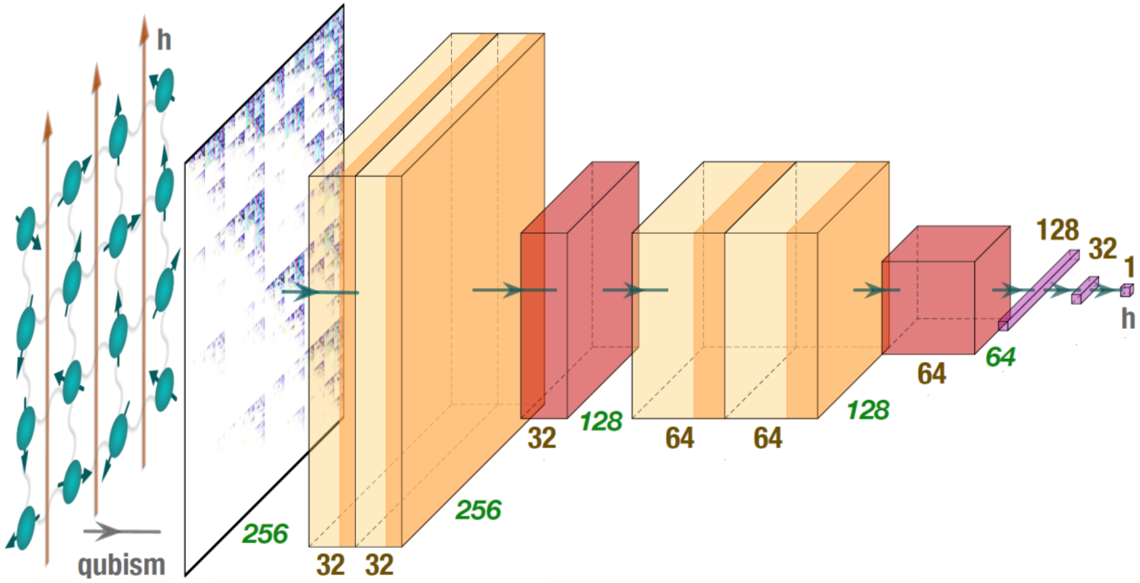
Deep Learning Quantum States For Hamiltonian Predictions

Shi-Ju Ran

Capital Normal University



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Deep learning quantum states for Hamiltonian predictions

Xinran Ma,[1] Z. C. Tu,[1] and Shi-Ju Ran[2,*]

[1]*Department of Physics, Beijing Normal University, Beijing 100875, China*
[2]*Department of Physics, Capital Normal University, Beijing 100048, China*

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Xiran Ma

Prof Z.C Tu

北京師範大學
BEIJING NORMAL UNIVERSITY

国家自然科学基金委员会
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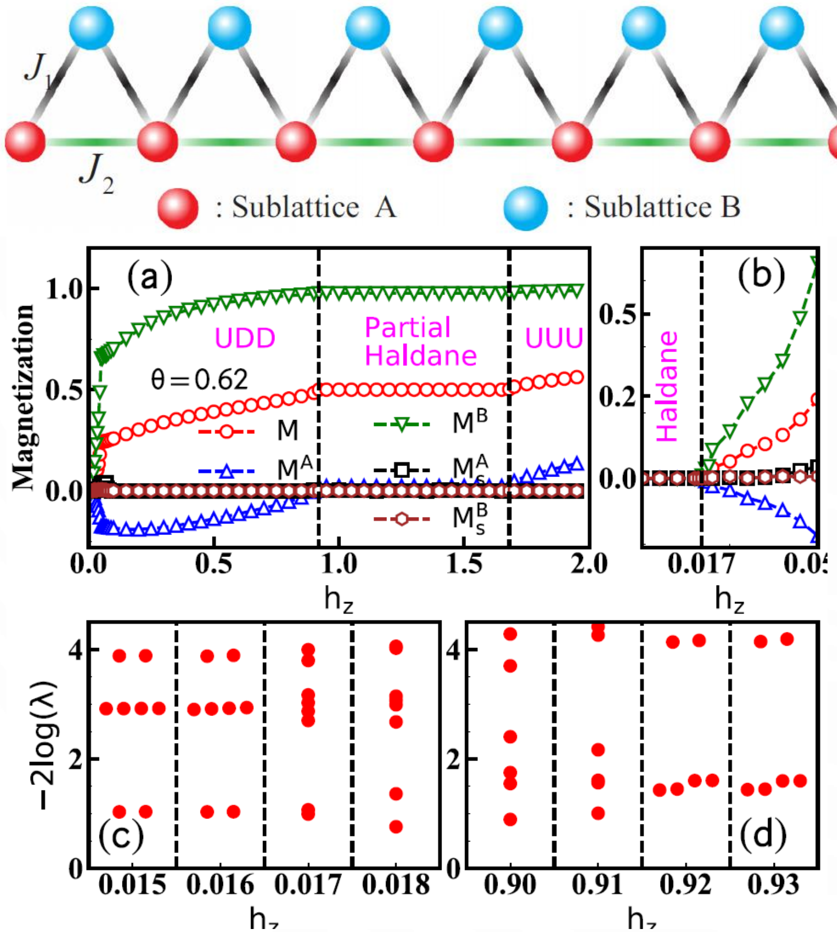
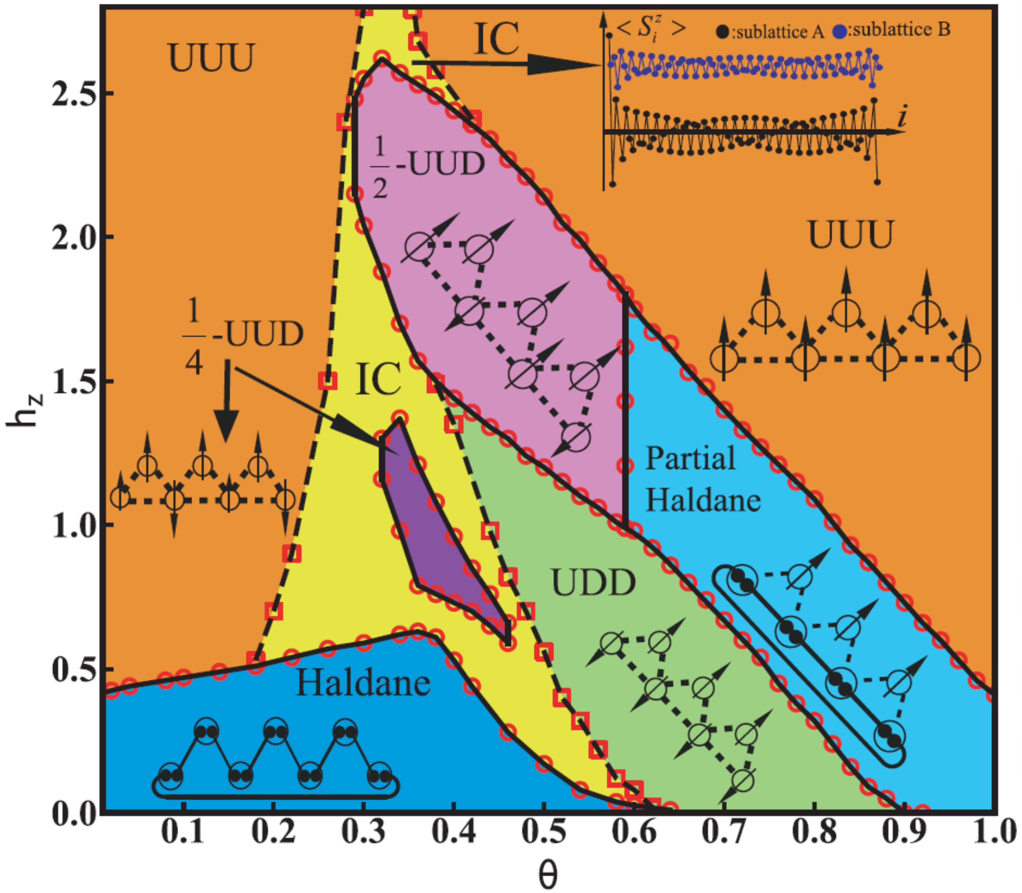
Interactions in quantum many-body systems lead to fruitful novel phenomena

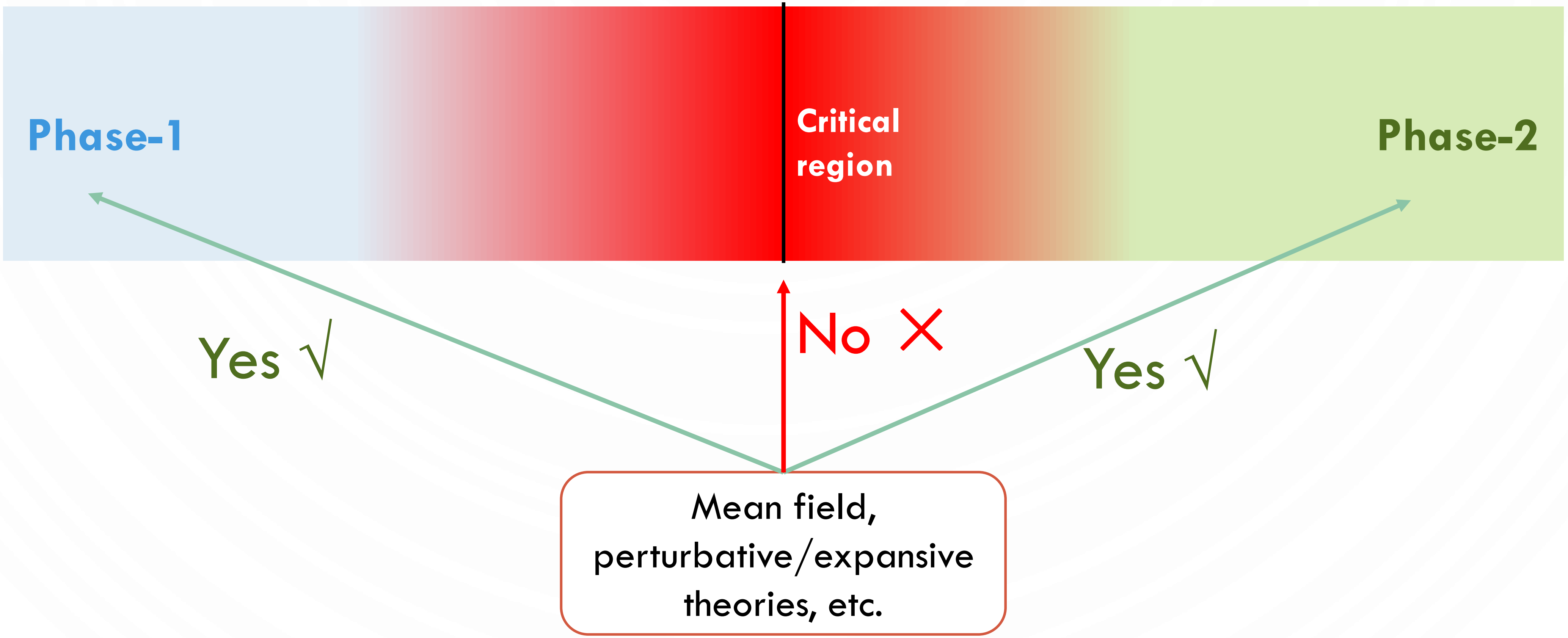
Example: spin-1 antiferromagnetic Heisenberg sawtooth chain (simulated with DMRG)

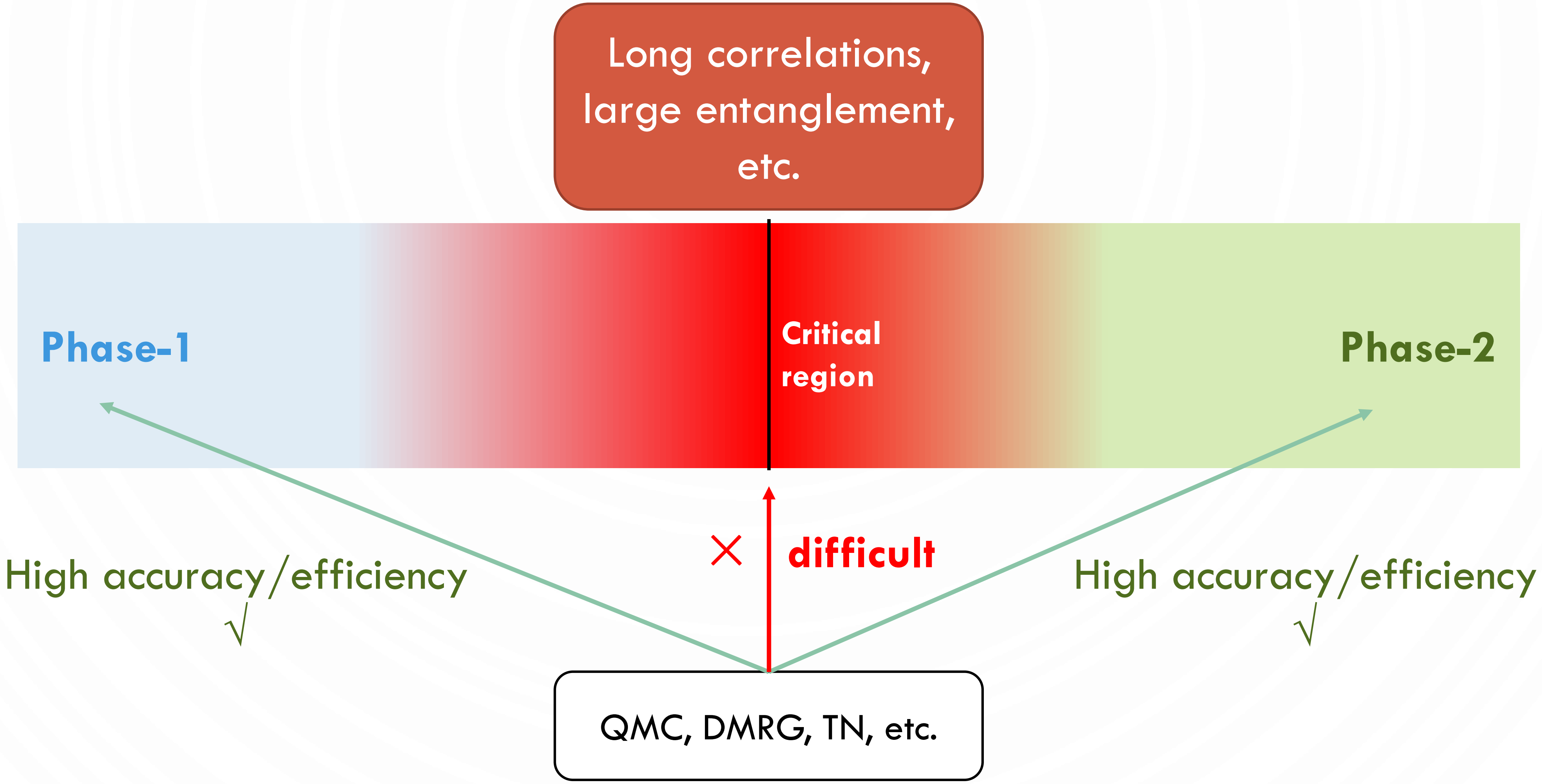




Yuan Yang, Shi-Ju Ran*, Xi Chen, Zhengzhi Sun, Shou-Shu Gong, Zhengchuan Wang*, Gang Su*. *Reentrance of Topological Phase in Spin-1 Frustrated Heisenberg Chain*. Phys. Rev. B **101**, 045133 (2020)

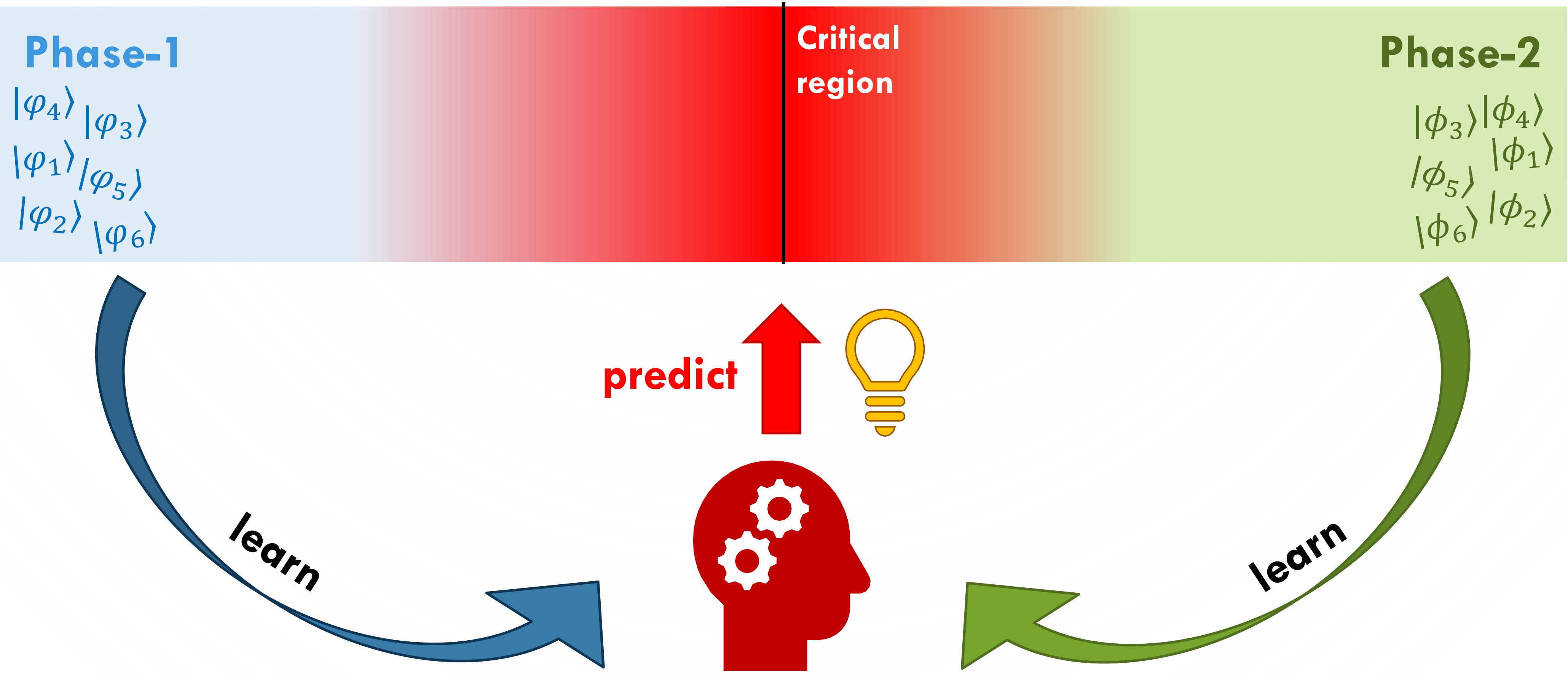
Challenges in simulating quantum many-body systems





Long correlations, large entanglement, etc.
Phase-1
Critical region
Phase-2
High accuracy/efficiency √
× difficult
High accuracy/efficiency √
QMC, DMRG, TN, etc.

Learn the critical vicinity?



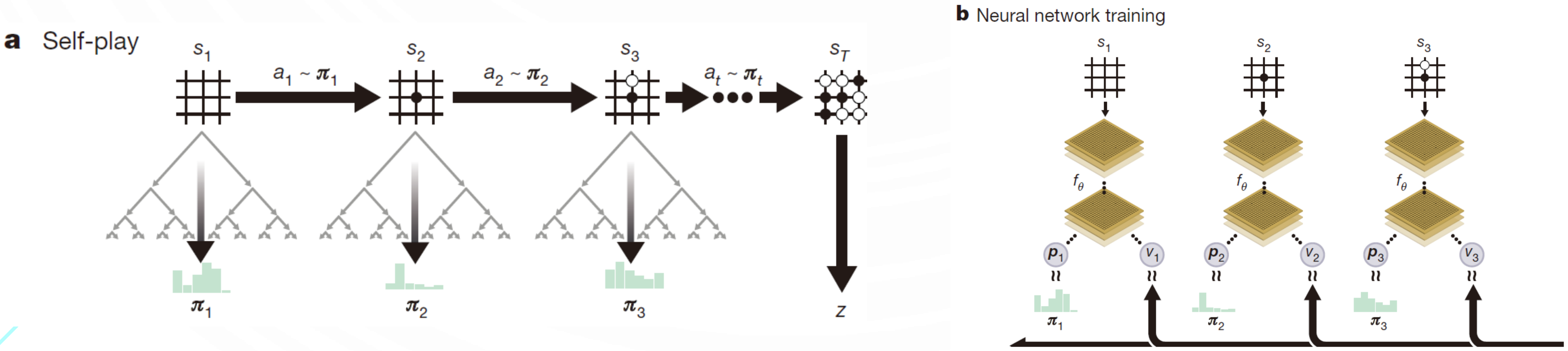
Neural network is a powerful machine learning model

ARTICLE

doi:10.1038/nature24270

Mastering the game of Go without human knowledge

David Silver[1]*, Julian Schrittwieser[1]*, Karen Simonyan[1]*, Ioannis Antonoglou[1], Aja Huang[1], Arthur Guez[1], Thomas Hubert[1], Lucas Baker[1], Matthew Lai[1], Adrian Bolton[1], Yutian Chen[1], Timothy Lillicrap[1], Fan Hui[1], Laurent Sifre[1], George van den Driessche[1], Thore Graepel[1] & Demis Hassabis[1]



Can NN solve physical problems in a **data-driven** way?

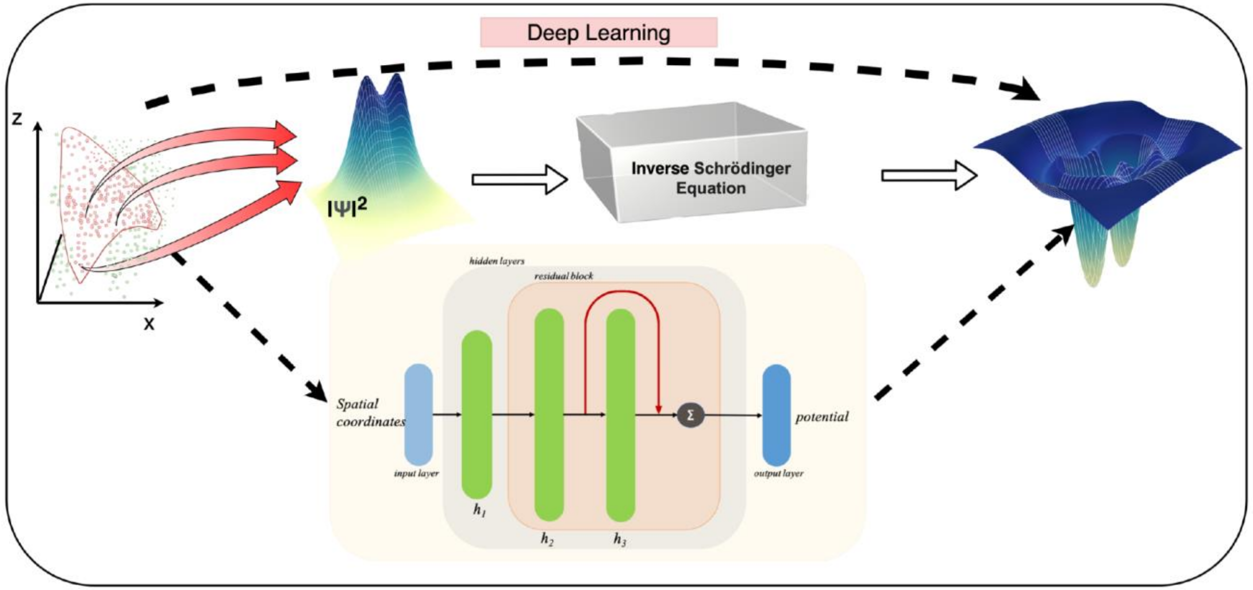
- Opportunities to solve a new kind of problems in quantum physics, such as the inverse problems of solving Hamiltonian given the states

Learning Potentials of Quantum Systems using Deep Neural Networks

Arijit Sehanobish,*[1] Hector H. Corzo,*[2] Onur Kara,[3] David van Dijk[1]

[1] Internal Medicine (Cardiology) and Computer Science, Yale University
{arijit.sehanobish, david.vandijk}@yale.edu
[2] Center for Chemical Computation and Theory
University of California, Merced
hhcorzo@gmail.com
[3] Hindsight Technology Solutions
okara83@gmail.com

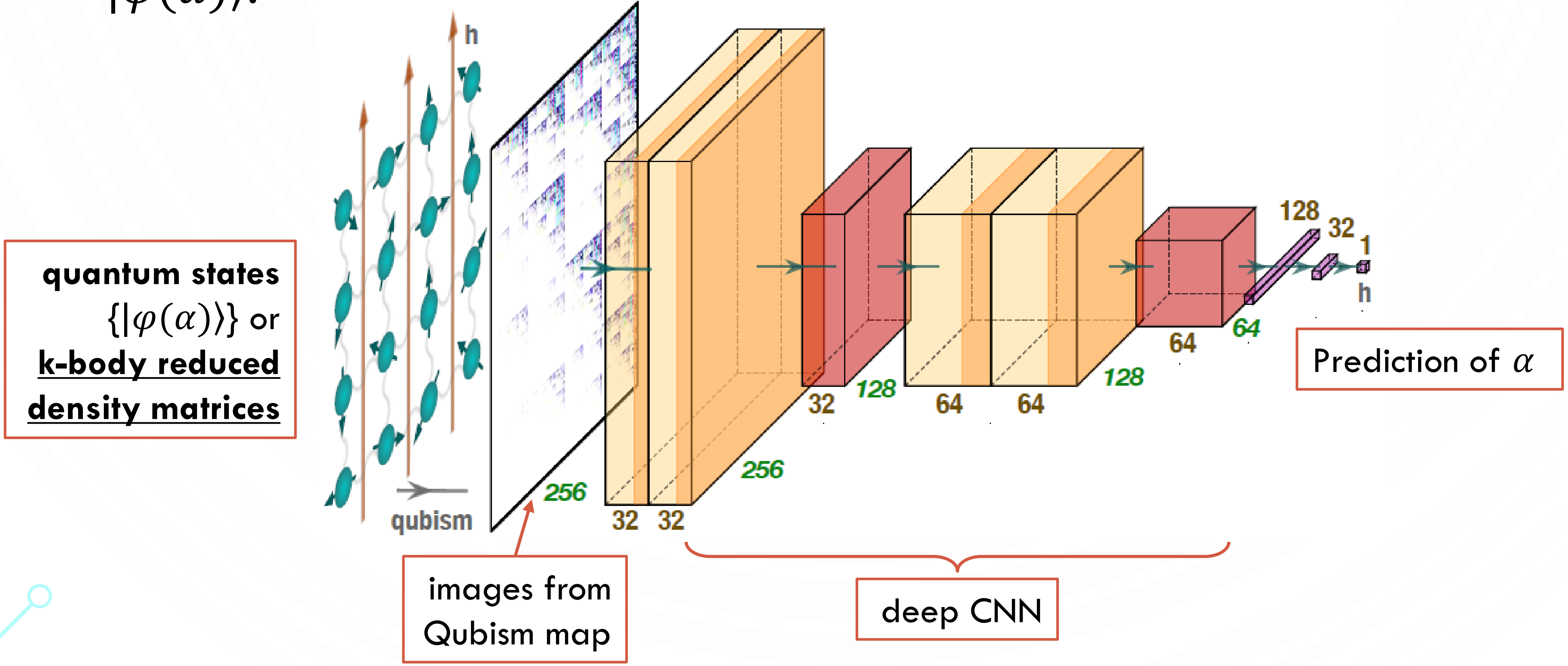
arXiv:2006.13297



QubismNet for many-body Hamiltonian predictions

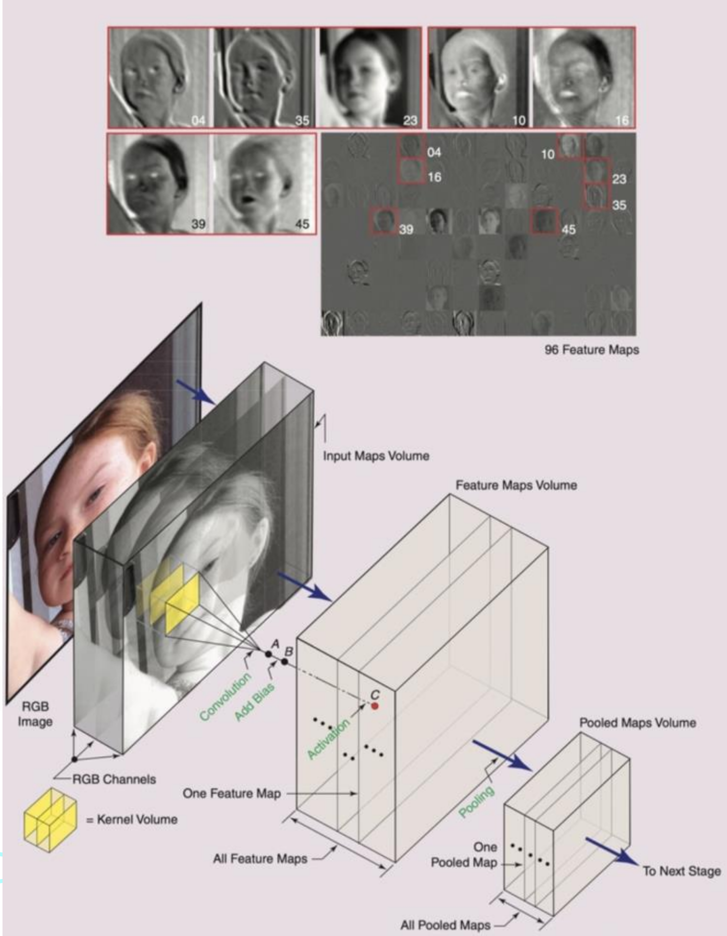
Basic ideas

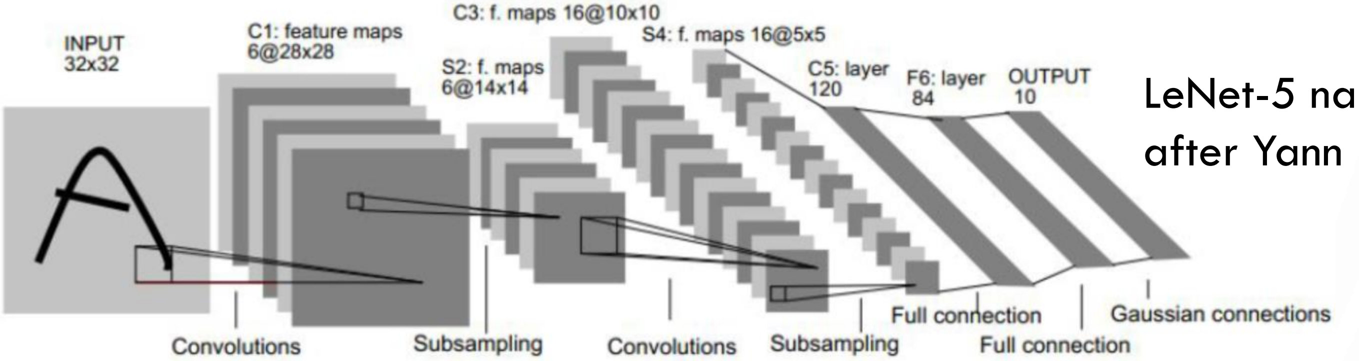
- Main target: considering the Hamiltonian $\hat{H}(\alpha)$ parametrized by α (e.g., coupling constant, magnetic field, etc.), predict α given the ground state $|\varphi(\alpha)\rangle$.



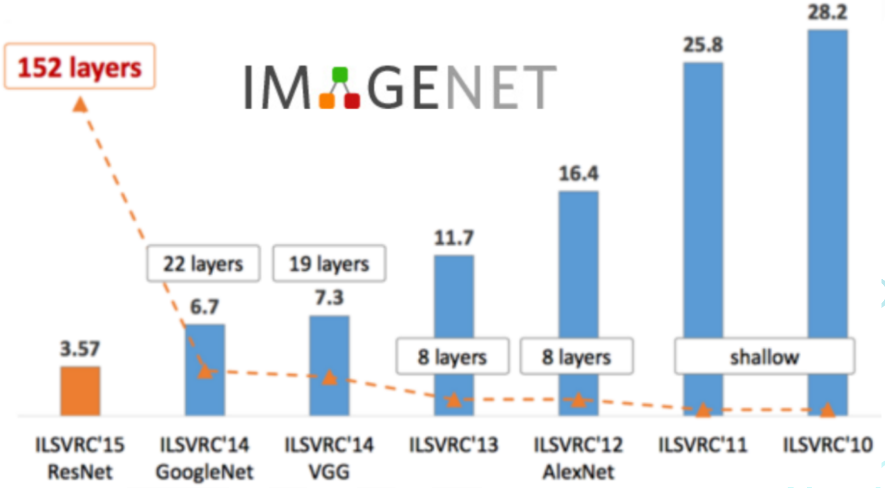
Convolutional neural network

- One of the most powerful machine learning model for processing images





LeNet-5 named after Yann LeCun



What is Qubism?

- One-to-one mapping from quantum states to images

New Journal of Physics
The open-access journal for physics

Qubism: self-similar visualization of many-body wavefunctions

Javier Rodríguez-Laguna[1,2,5], **Piotr Migdał**[1], **Miguel Ibáñez Berganza**[3], **Maciej Lewenstein**[1,4] **and Germán Sierra**[3]
[1] ICFO—Institute of Photonic Sciences, Castelldefels, Barcelona, Spain
[2] Mathematics Department, Universidad Carlos III de Madrid, Spain
[3] IFT—Instituto de Física Teórica, UAM/CSIC, Cantoblanco, Madrid, Spain
[4] ICREA—Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain
E-mail: javier.rodriguez@icfo.es

New Journal of Physics **14** (2012) 053028 (30pp)

$$\hat{H}(h) = J \sum_{\langle i,j \rangle} \hat{S}_i^z \hat{S}_j^z - h \sum_{k=1}^{L} \hat{S}_k^x$$ Quantum Ising

$$\hat{H}(J_z) = \sum_{\langle i,j \rangle} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + J_z \hat{S}_i^z \hat{S}_j^z).$$ XXZ

$$\hat{H}(h) = \sum_{\langle i,j \rangle} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y) + h \sum_{k=1}^{L} \hat{S}_k^z$$ XY

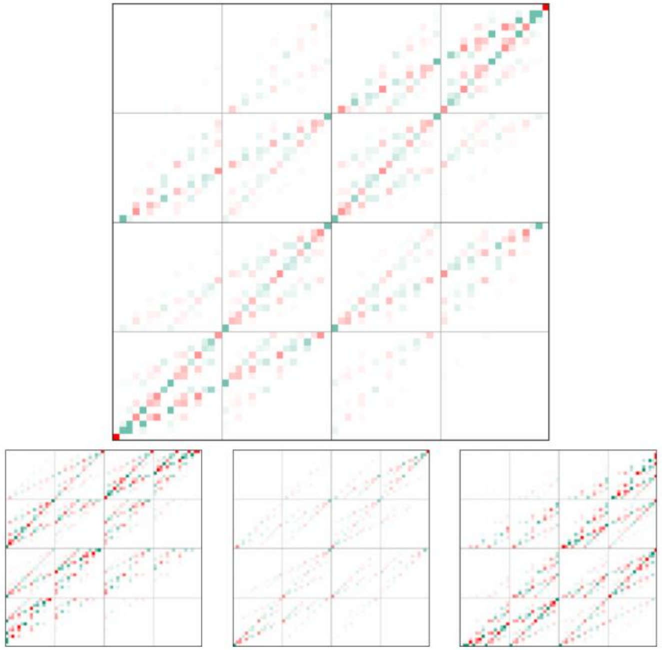
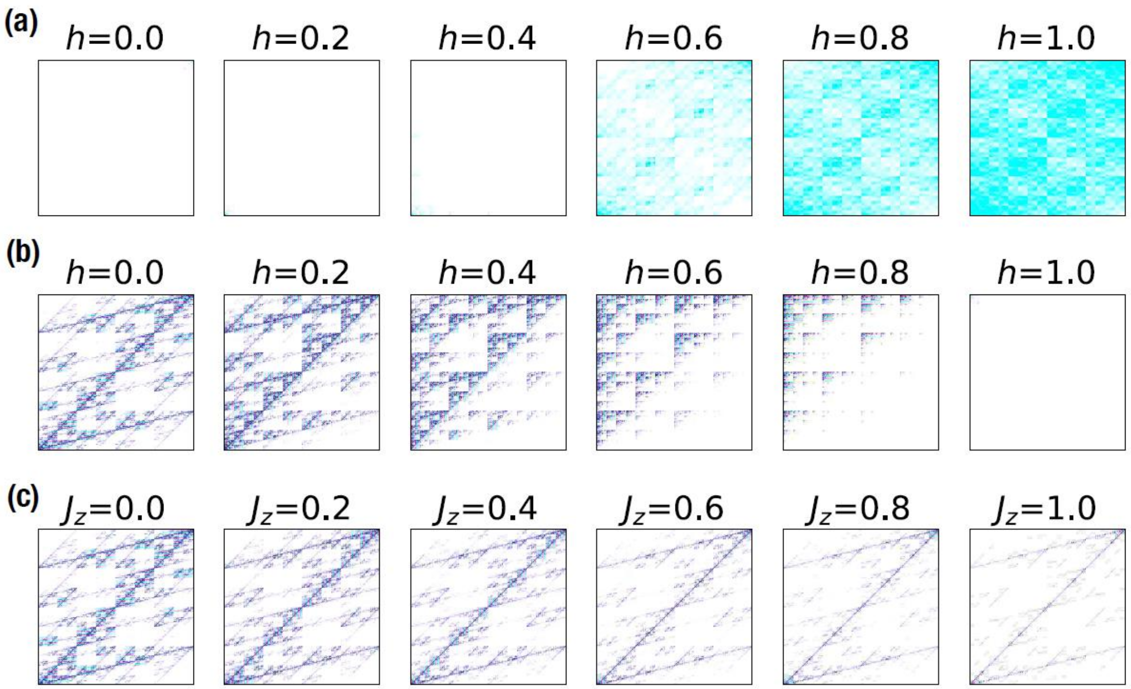


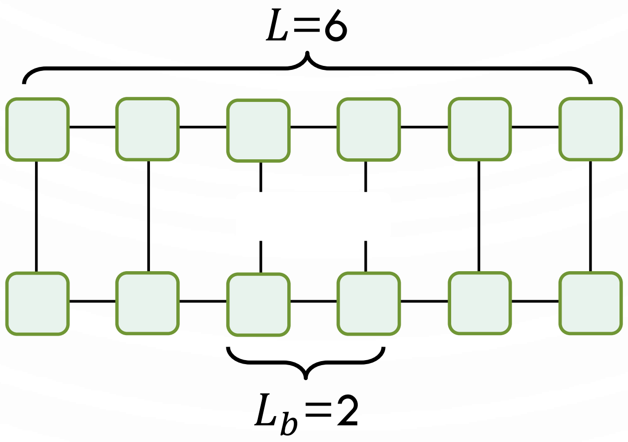
Figure 4. Top: ground state of the 1D spin-1/2 AF Heisenberg model with PBC for 12 spins. Bottom: the lowest energy excitations, which make up a triplet. White means zero probability, color intensity reflects the modulus of the wavefunction amplitude, whereas the hue marks the phase.



Illustrations of the images by the Qubism map from the ground states of the QIM, XY, and XXZ models

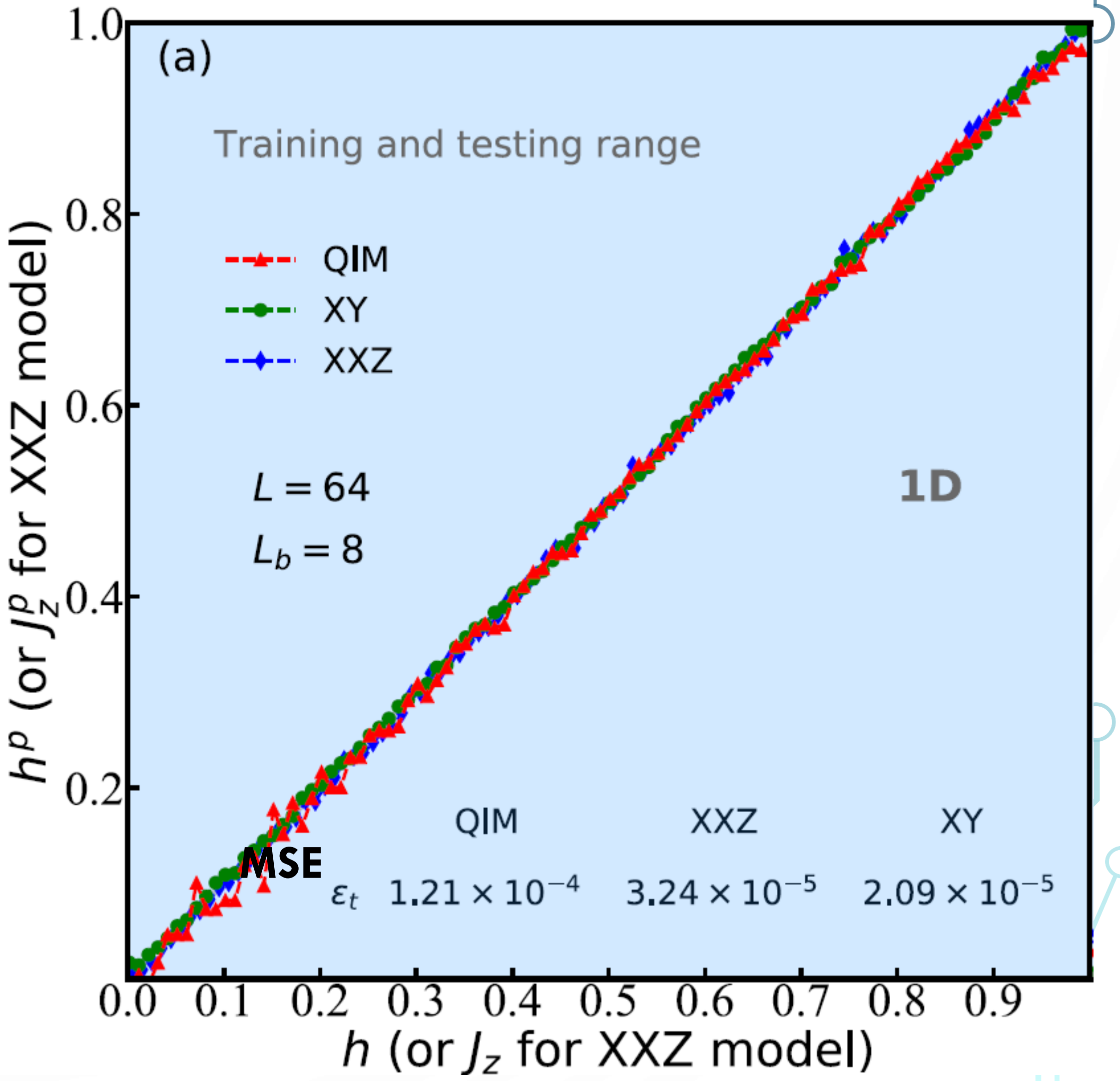
Learning from reduced density matrix

- One drawback of Qubism: the cost increases **exponentially** with the system size;
- Learn from **the reduced density matrix** (RMD) of a bulk with size $L_b \ll L$ (L=64 in practice);
- The ground states with large L are represented by **matrix product states** (MPS).



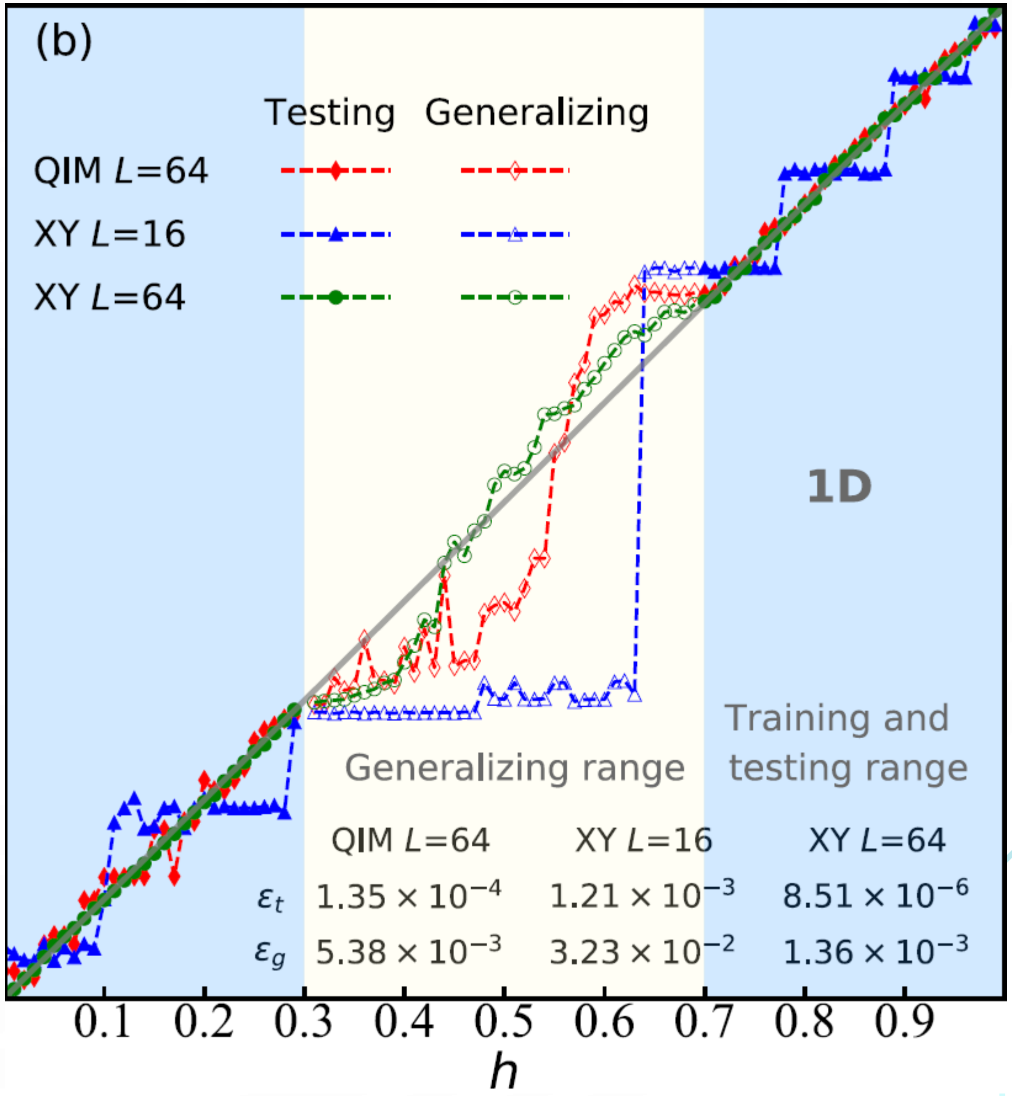
Training and testing accuracies on quantum chains

- Samples in the training set (to optimize the parameters in the NN) ;
- MSE: $\frac{1}{\mathrm{N}}\sum_{n=1}^{N}|h_n^p - h_n|^2$
- MSE error for the samples in the testing set (**independently and identically** distributed as the training samples, but are not fed to the NN) is small ~O(10^{-4}~10^{-5})
- On QIM, criticality seems to have no effects to the predictions

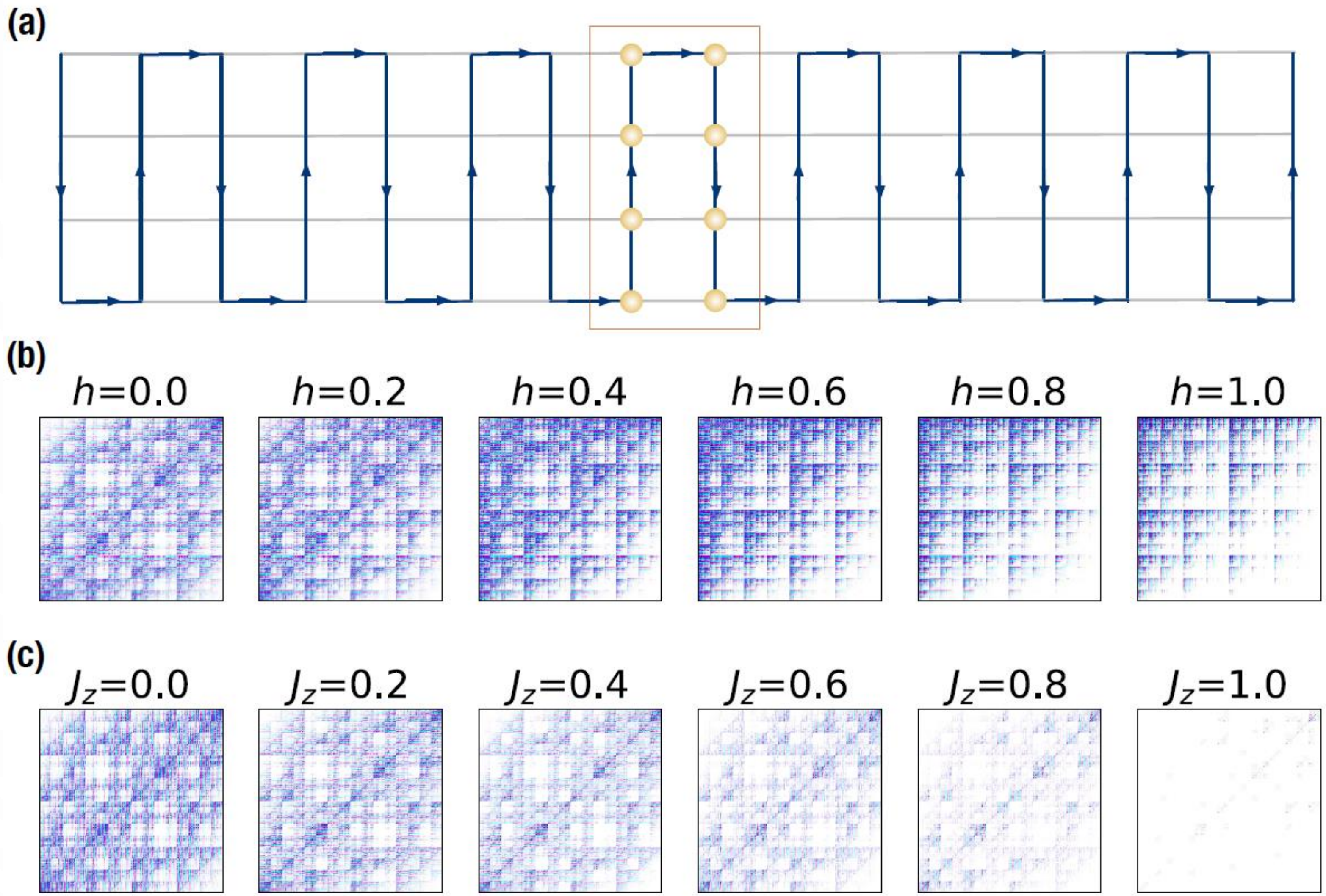


Generalization power on 1D chains

- **Generalization set**: the states from **different region** (light yellow) from the training and test sets (light blue);
- We take the width for taking the generalizing set $\delta = 0.4$.
- When L is small, **stages** appears in the prediction curve, due to the **energy gaps** of the eigenstates of the Hamiltonian.
- The gaps are suppressed by **increasing L**, and the accuracies will also be improved.
- For the quantum Ising mode, the NN **learns from the states away from the critical point**, and can still **well predict the magnetic field of the states in the critical vicinity**;



Generalization power on 2D systems

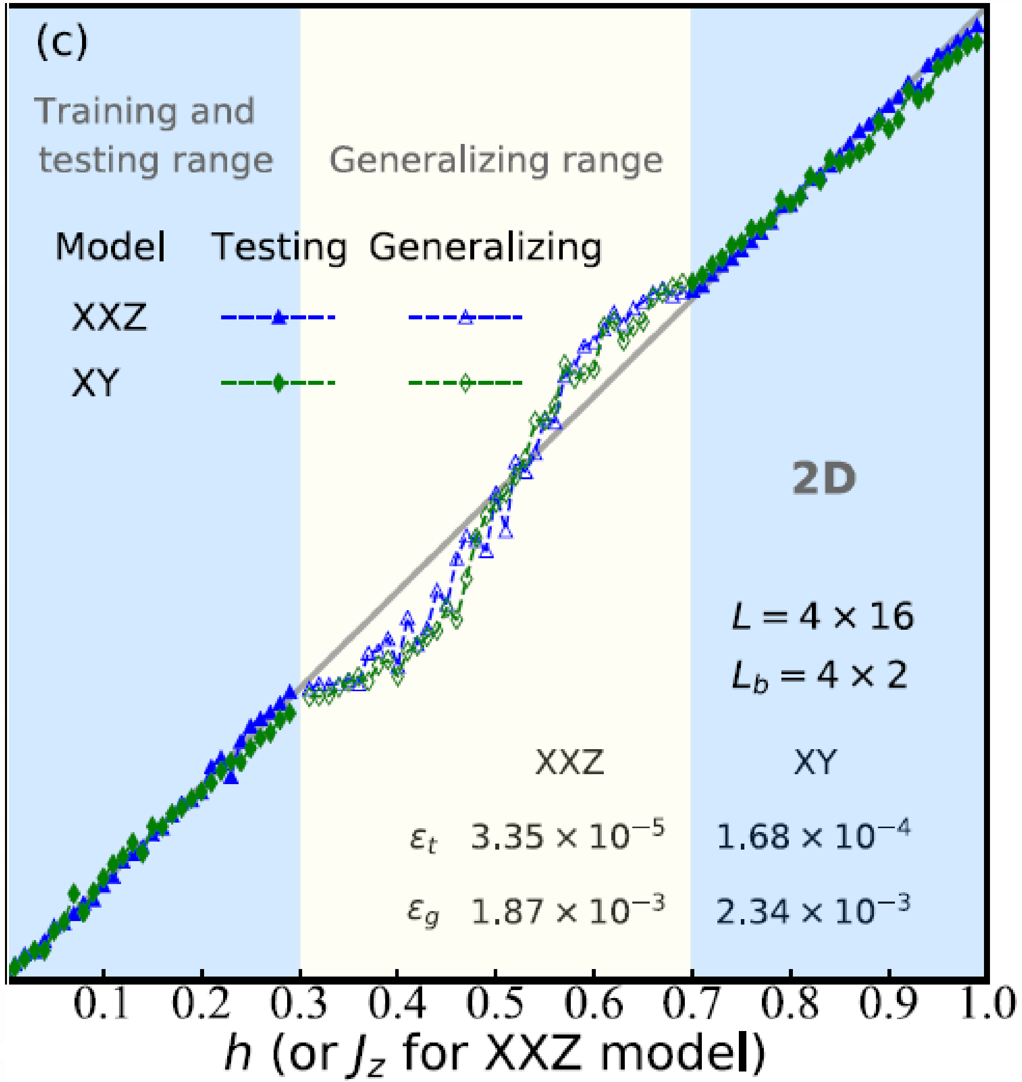


XY

XXZ

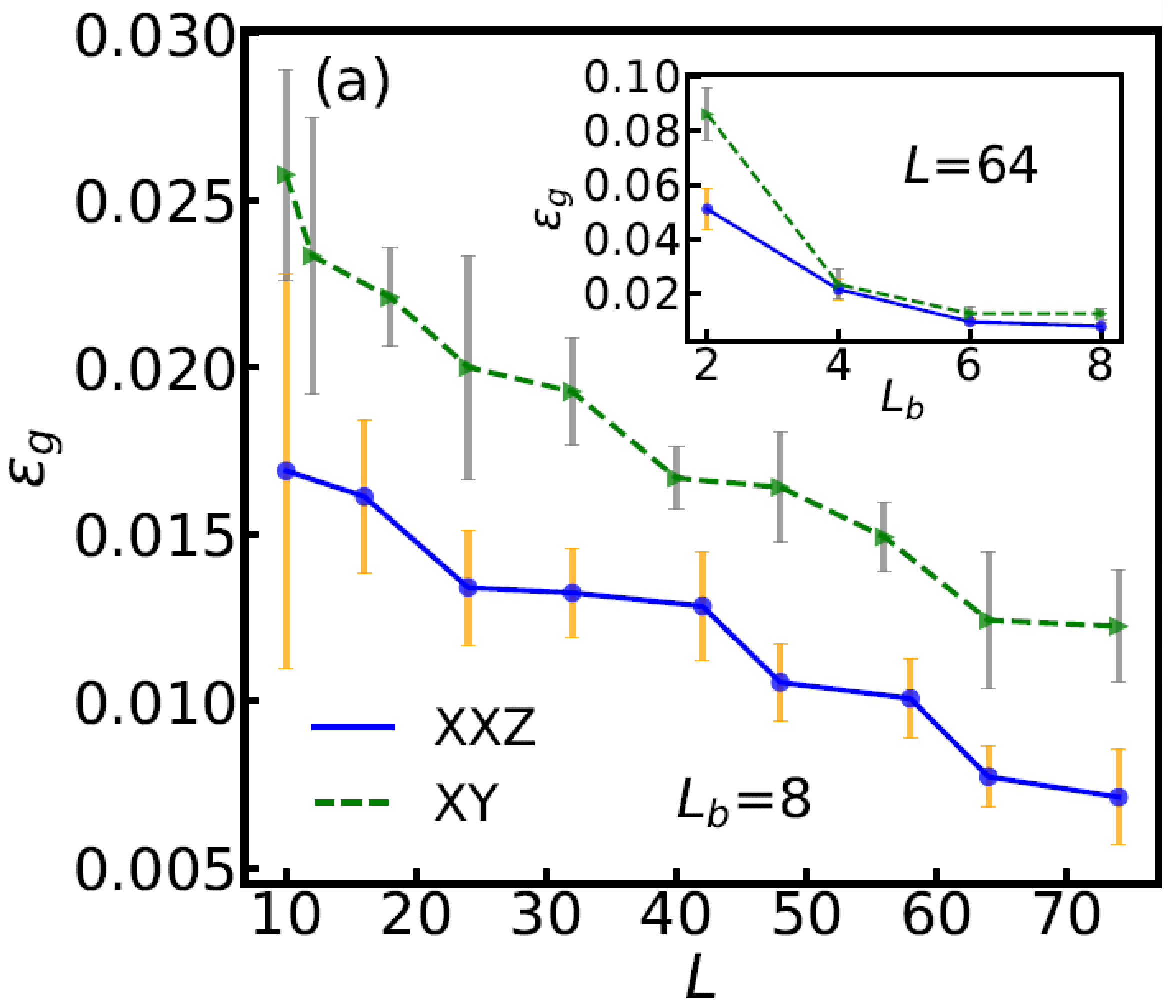
Generalization power on 2D systems

- Similar accuracies are achieved on the XXZ and XY models on the finite-size square lattice.



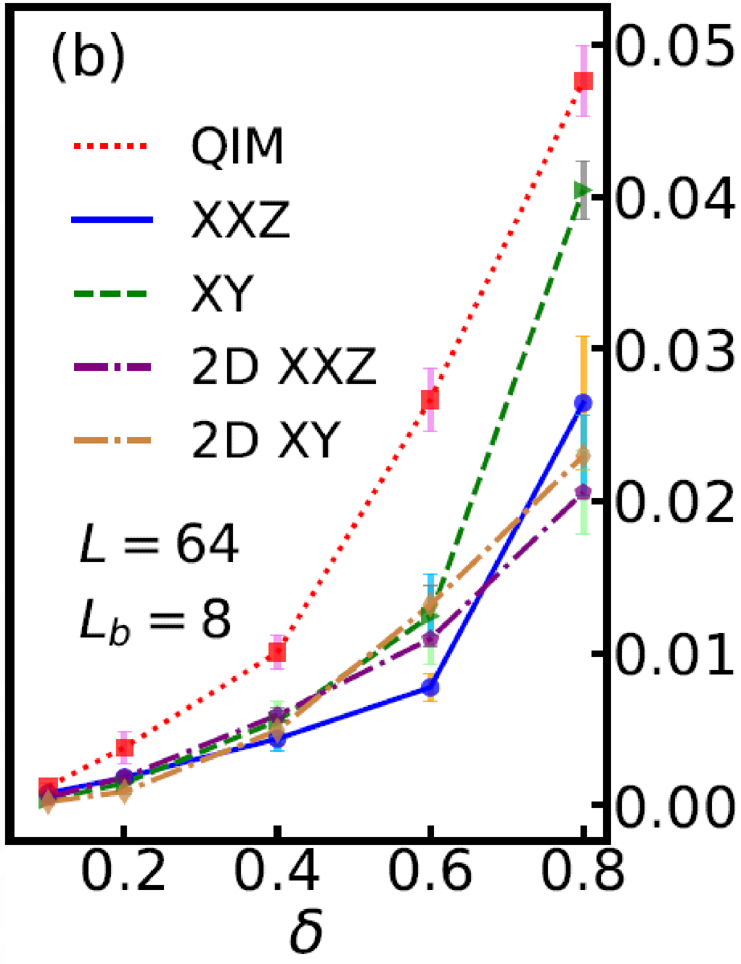
Size dependence of generalization power

- By fixing L_b=8, both the **error** and **the strength of the fluctuations** for the generalization set decreases with **L**.
- By fixing L=64, both the **error** and **the strength of the fluctuations** for the generalization set decreases with $\mathbf{L_b}$.
- The error converges for L_b~6-8, indicating the correlation length of the states.



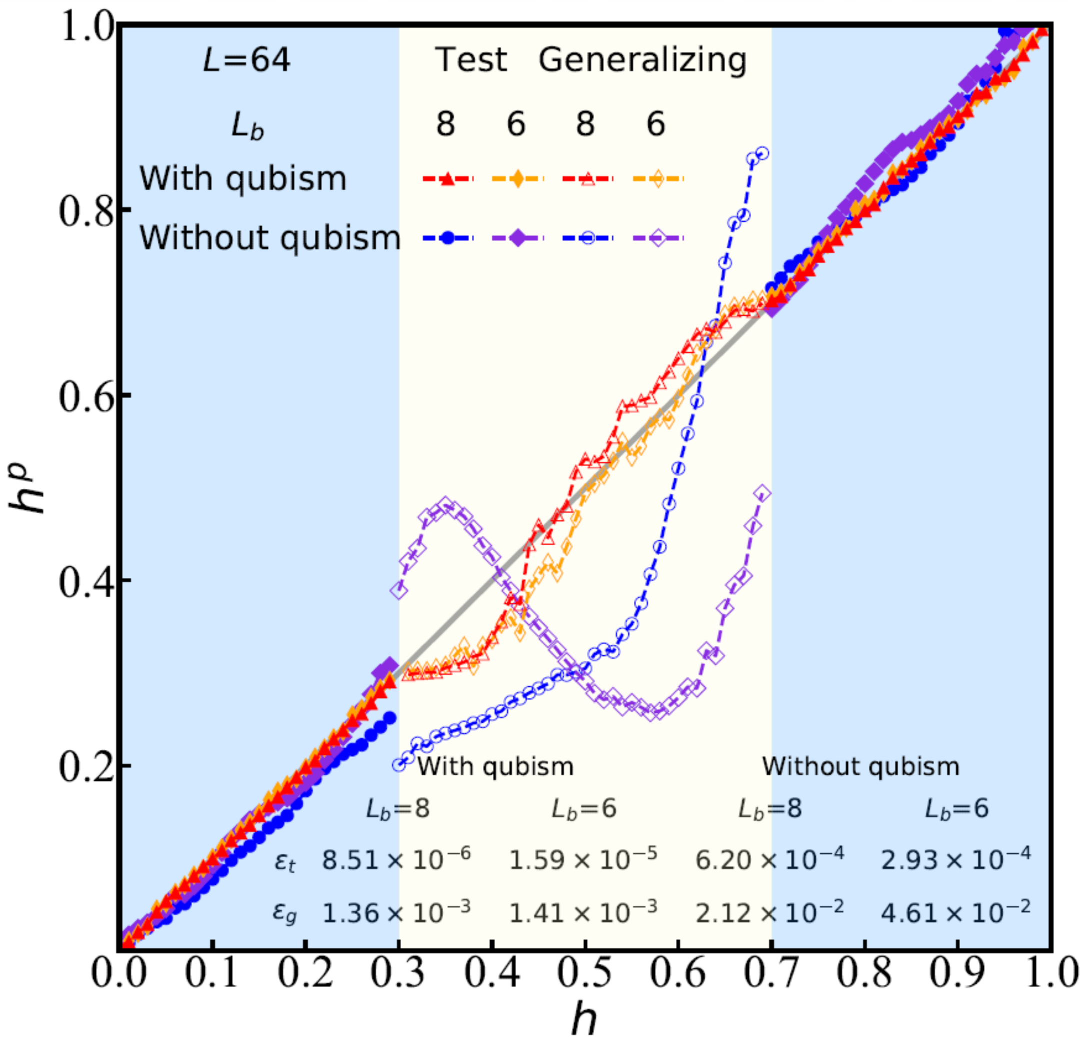
Generalization power for different parameter gaps

- The generalization error increases with the parameter gap δ (the width of the region where we sample the generalization set).
- But at most, the error reaches $\varepsilon_g \sim 0.05$ for $\delta = 0.8$. For small δ, we have $\varepsilon_g \sim O(10^{-3})$ or less.



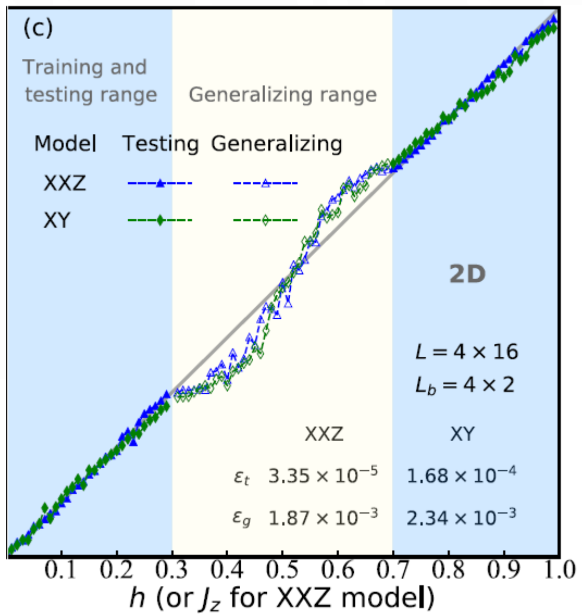
1D CNN performs more poorly than 2D CNN

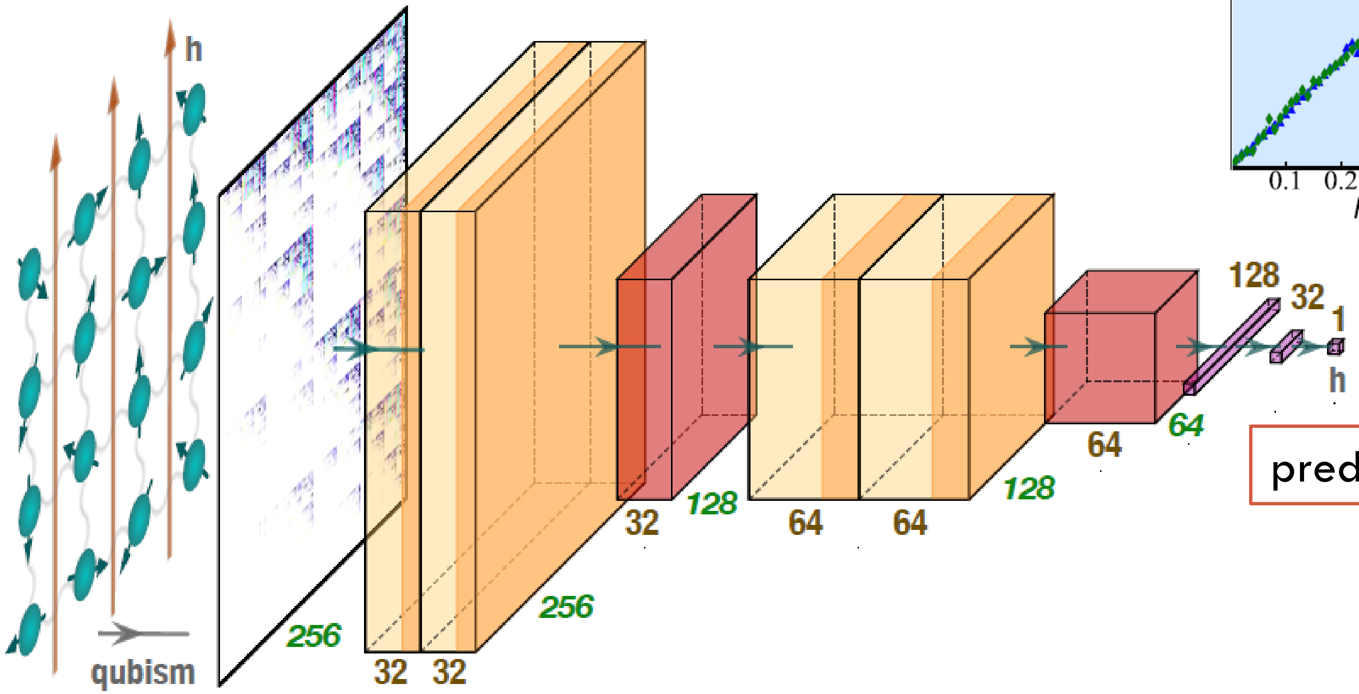
- 1D CNN with Qubism map performs obviously more poorly than 2D CNN with Qubism map, particularly for the generalization set.
- This benefits from both the Qubism map and the superior power of CNN for processing 2D images.



Summary

excellent training, testing, and generalization powers





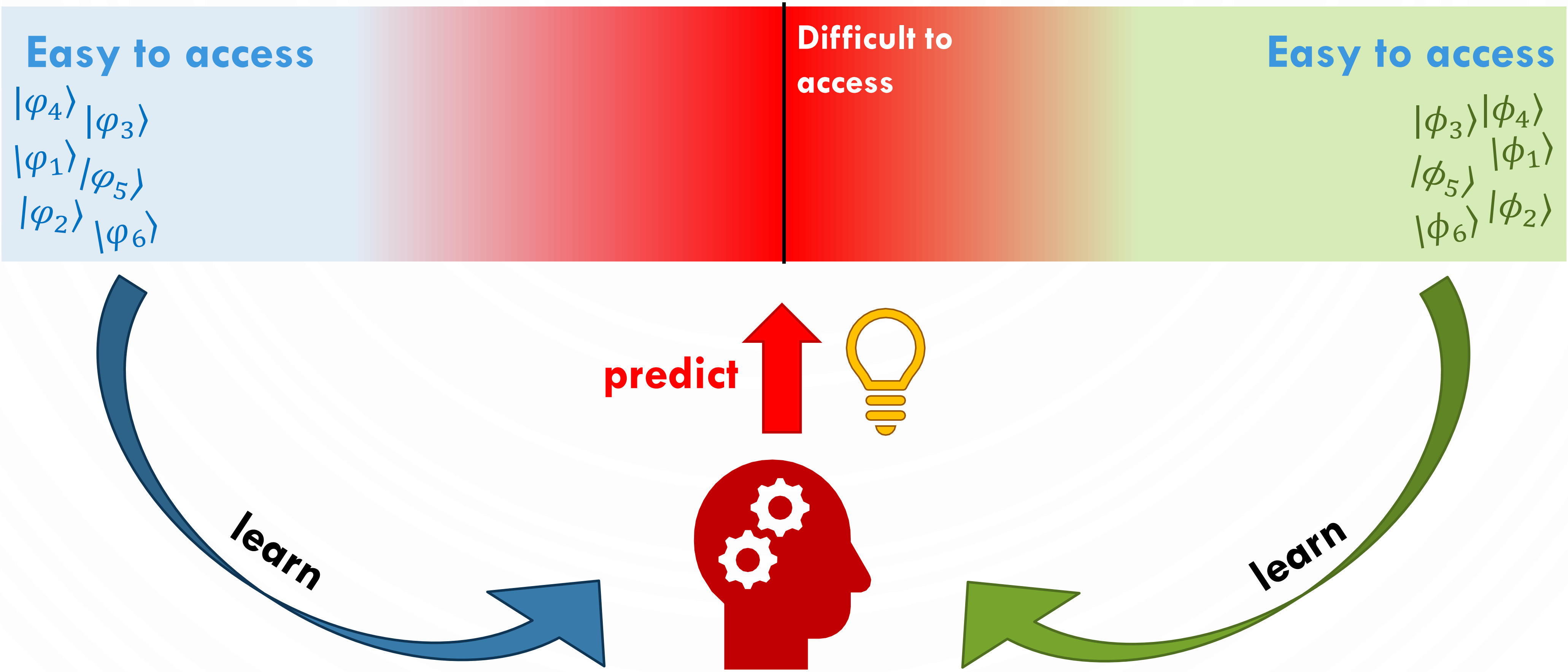
quantum states $\{|\varphi(\alpha)\rangle\}$

images from Qubism map

deep CNN

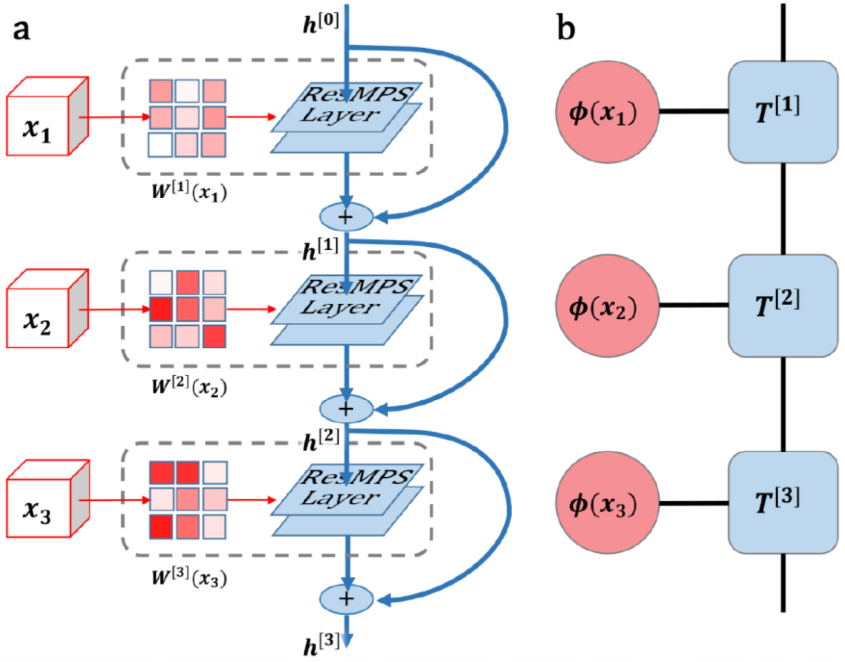
prediction of α

Perspective I:
What else can be learned beyond parameters?



Perspective II: TN machine learning

- TN is a young **quantum-inspired machine learning model**, such as supervised learning by MPS (E. Stoudenmire and D. J. Schwab, NIPS 2016).
- For machine learning, neural network (NN) still exhibits obvious advantages on the powers of expression and, particularly, **generalization**.



Model	MMIST train	MMIST test	Fashion-MMIST train	Fashion-MMIST test
MPS machine [28]	1.0000	0.9855	0.99	0.88
Unitary tree TN [9]	0.98	0.95	-	-
Tree curtain model [35]	-	-	0.9538	0.8897
Bayesian TN [15]	-	-	0.8950	0.8692
EPS-SBS [7]	-	0.9885	-	0.886
PEPS [17]	-	-	-	0.883
CNN-PEPS [17]	-	-	-	0.912
AlexNet [36]	-	-	-	0.8882
ResNet [36]	-	-	-	0.9339
sResMPS(+dropout)	1.0000	0.9898	0.9920	0.9076
aResMPS(+ReLU,+dropout)	1.0000	0.9900	0.9999	0.9146

Nonlinear TN model

Ye-Ming Meng, Jing Zhang, Peng Zhang, Chao Gao, and Shi-Ju Ran, arXiv:2012.11841.

Thank you for your attention!

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