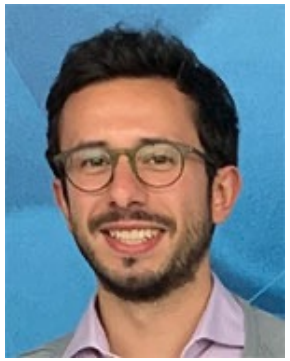
Quantum phase detection generalization from marginal quantum neural network models

Keypoint:

using quantum convolutional neural network we study the phase diagram of the Axial Next Nearest Neighbor Ising (ANNNI) model. We train on simplified and integrable models, obtaining promising generalization performance.

Paper:
Monaco, Kiss, Mandarino, Vallecorsa, Grossi, arXiv: 2208.08748 (2022)



Michele Grossi, PhD

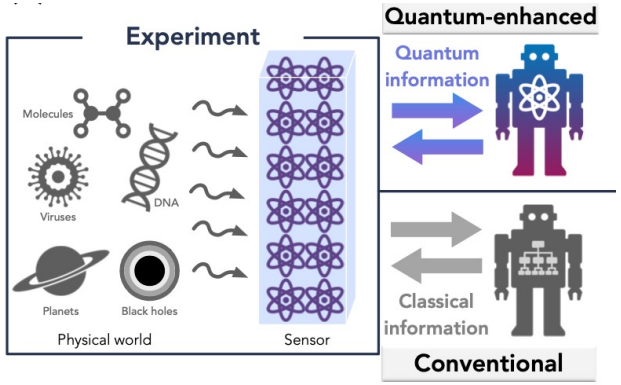
CERN QTI Quantum Computing Scientist

Quantum Computing for many body problems (QCMB)
IJCLab, Paris , November 2022

Quantum machine learning for quantum data

$$\mathcal{H} = -J_1 \sum_{i=1}^{N} \sigma_x^i \sigma_x^{i+1} - \kappa\, \sigma_x^i \sigma_x^{i+2} - h\, \sigma_z^i$$

1. Work directly with quantum states.
2. Bypass any classical processing.



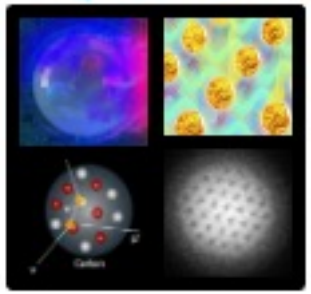
Huang, *et al., Science* **376**, 6598 (2022)

Task: Drawing phase diagrams

1. Supervised classification using a convolutional QNN using the groundstates as input data.
2. Advantageous since quantum states are exponentially hard to save classically.
3. Bottleneck: we need access to classical training labels! Interpolation does not work.

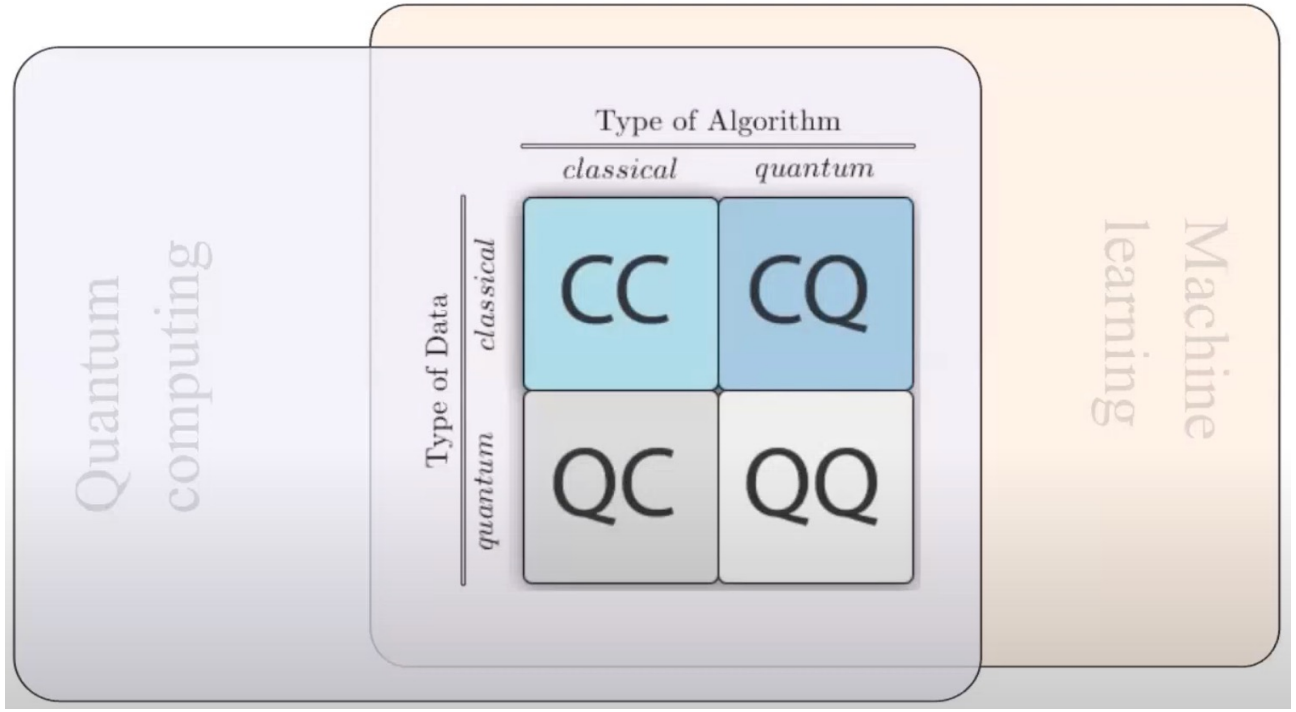
Cong, *et al., Nat. Phys.* **15**, 1273–1278 (2019)

- **QML in a nutshell**
- Data and model definition
- Results



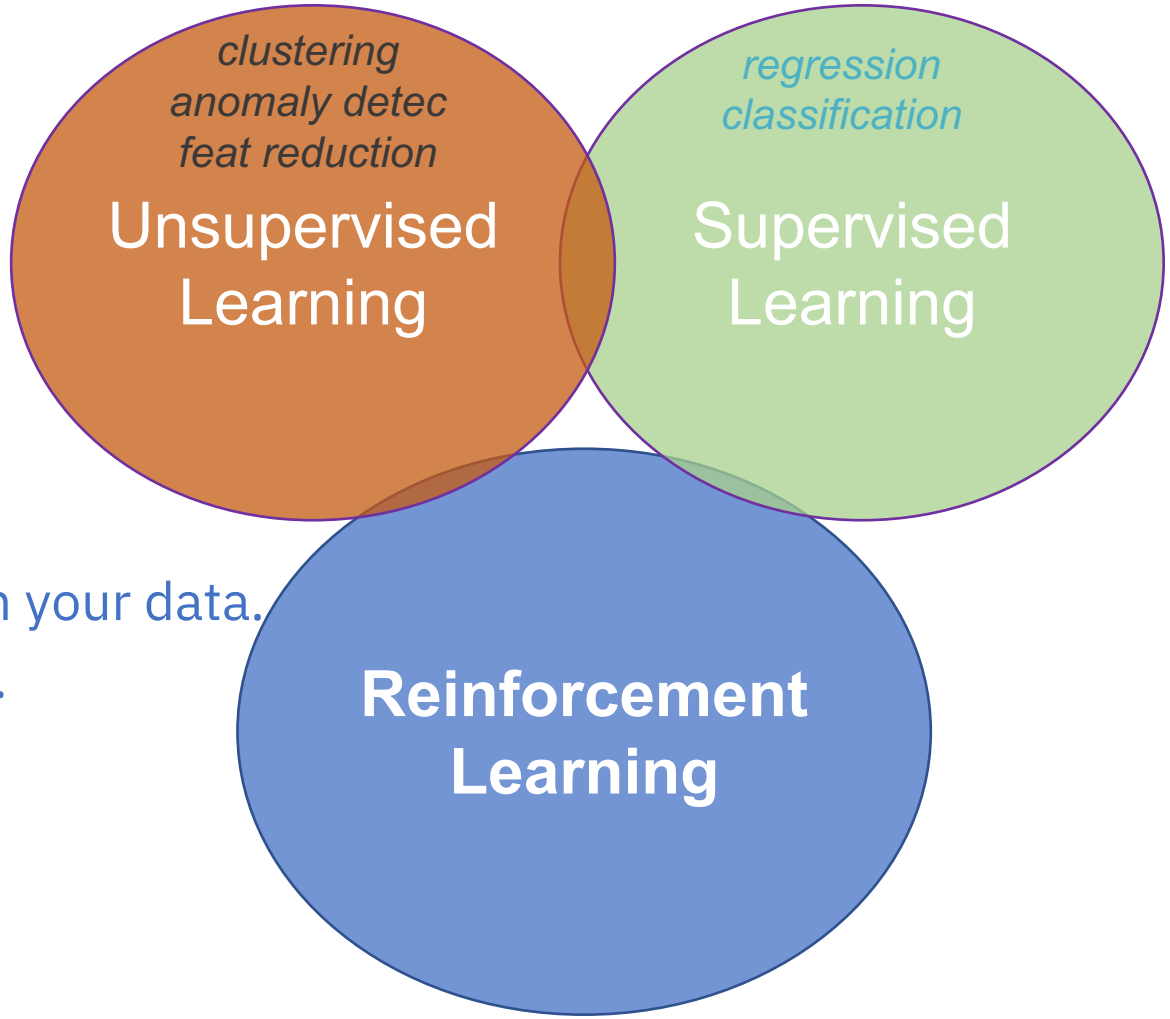
Quantum machine learning

- **Classical intractability**: what useful problems can we solve on a quantum computer that we cannot on a classical computer?
- **Innovation**: what new algorithms can we come up with?
- **Computational complexity**: how can we obtain certain speedups?
- Can quantum **supremacy** be proved with QML?



M.Schuld: QSI Seminar - Encoding Classical Data into Quantum States for ML

You got your data: what's next?



Supervised ML

Labeled data, i.e., data with defined output.

A model is trained giving this data and you have direct evaluation.

Unsupervised ML

Unlabeled data.

ML finds patterns in your data.

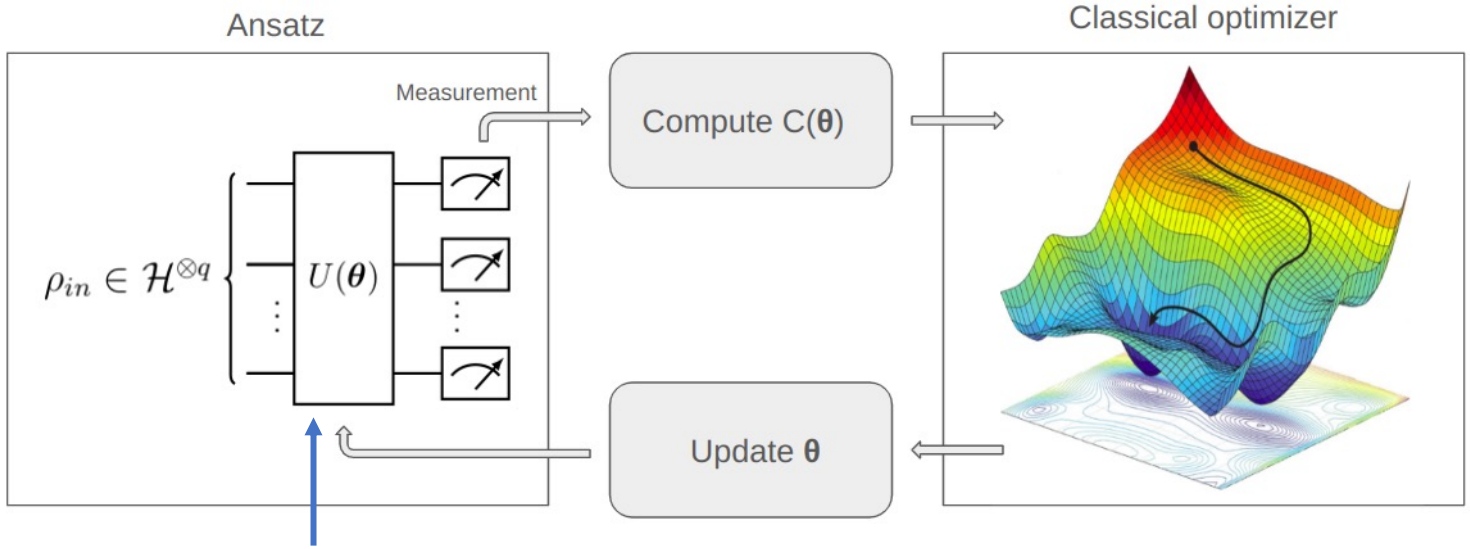
Indirect evaluation.

Quantum Computing

QML models implementations for NISQ

Variational algorithms - EXPLICIT

- Flexible parametric ansatz: design can leverage data symmetries[1,2]
- Can use **gradient-free** methods or **stochastic gradient-descent**
- **Data Embedding** can be **learned**
- **Better generalization[2,3]**



Parametrized circuit

A linear model in the quantum feature space!

1-A. Bogatskiy et al. "Lorentz group equivariant neural network for particle physics." PMLR, 2020

2-J. Meyer et al "Exploiting symmetry in variational quantum machine learning", https://arxiv.org/abs/2205.06217

3-S.Jerbi at all., Quantum Machine Learning Beyond Kernel Methods https://arxiv.org/abs/2110.13162

4- Glick, Jennifer R., et al. "Covariant quantum kernels for data with group structure." arXiv:2105.03406 (2021)

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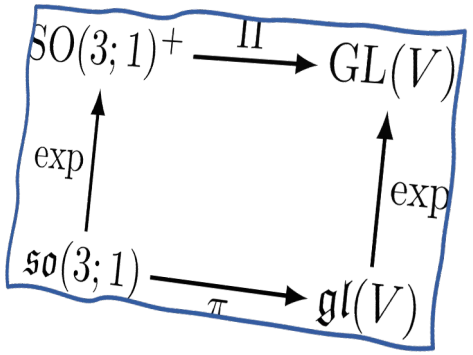
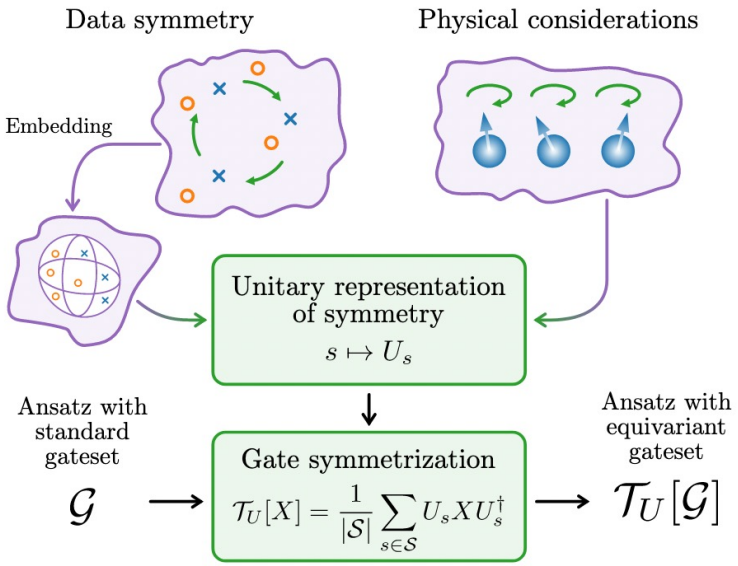
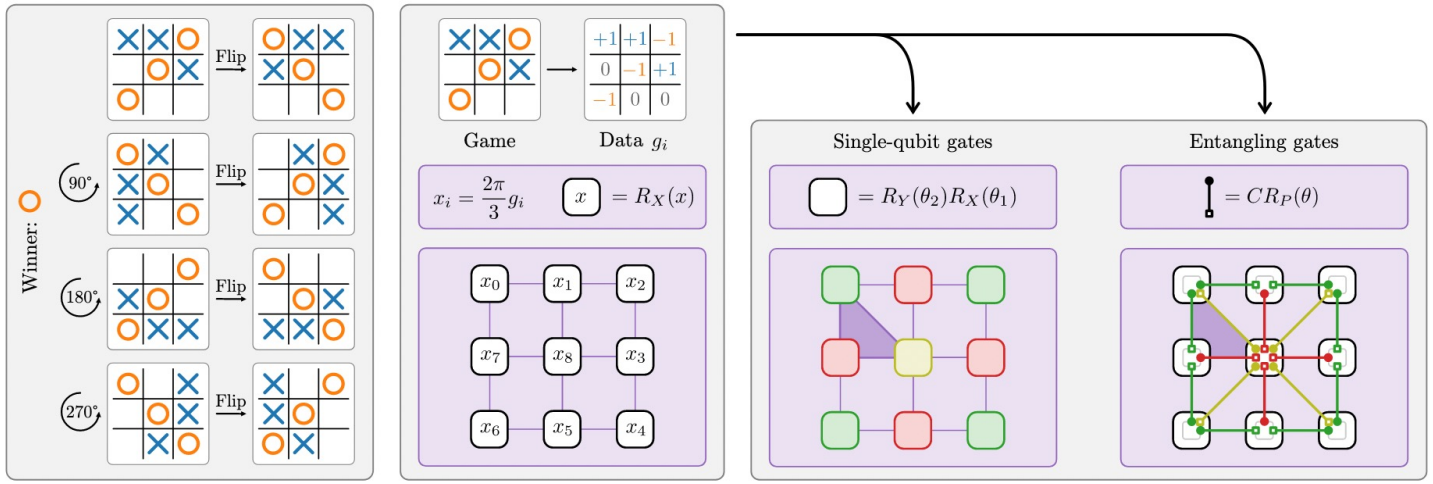


https://github.com/fizisist/LorentzGroupNetwork





A unitary representation of a symmetry group S can arise from data symmetries when the data points are suitably encoded or alternatively from physical considerations of a variational problem[2].

1-A. Bogatskiy et al. "Lorentz group equivariant neural network for particle physics." PMLR, 2020
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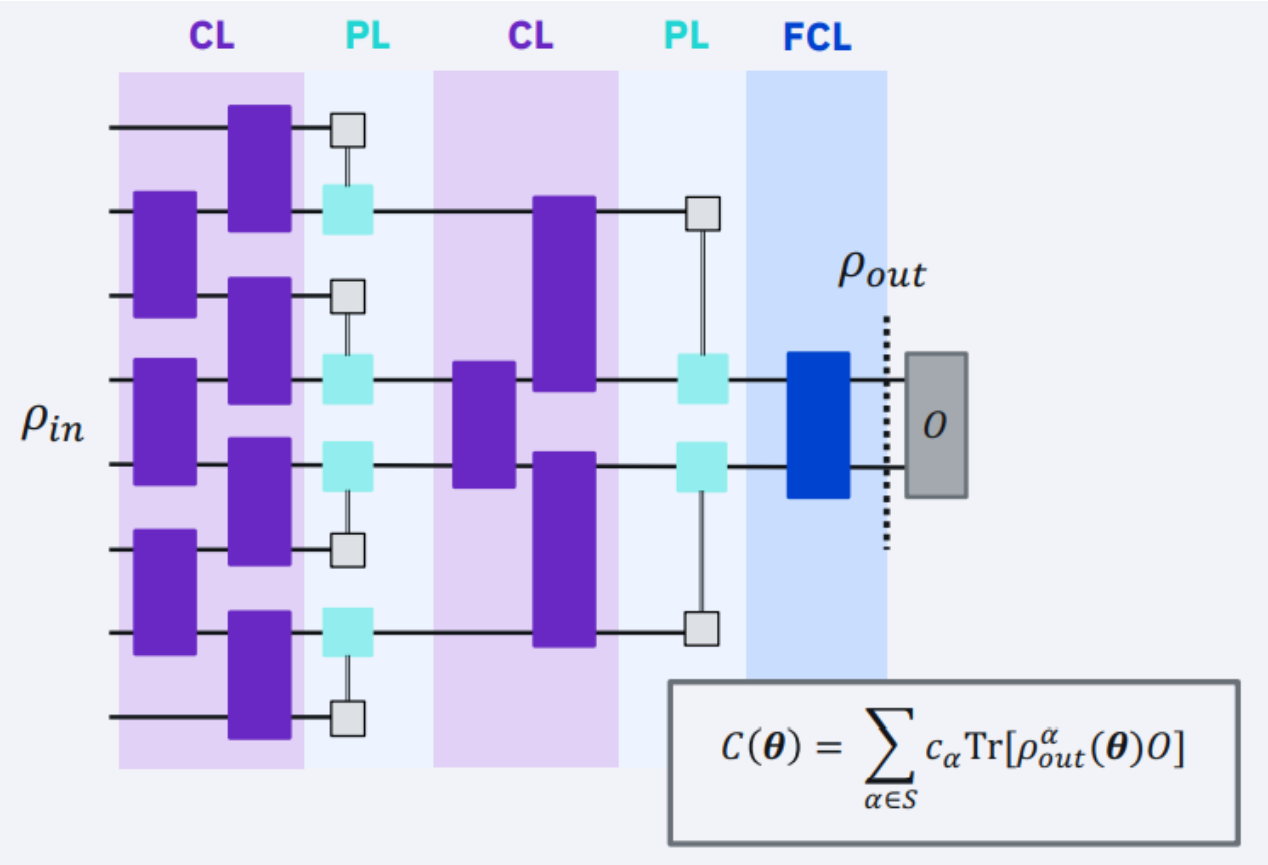
Quantum convolutional networks



- Can have as few as $O log(n)$ parameters
- Related to hierarchical quantum circuits like tree-tensor networks and multi-scale entanglement renormalization ansatz
- Can be used to analyse classical data or quantum states
- Quantum phase recognition, quantum error correction, entanglement detection, …
- QCNNs are “naturally” shallow

Grant et al., npj Quant. Inf. 4, 65 (2018)
I. Cong et al., Nature Physics 15, 1273 (2019)
Pesah et al., arXiv:2011.02966 (2020)

Open Problem

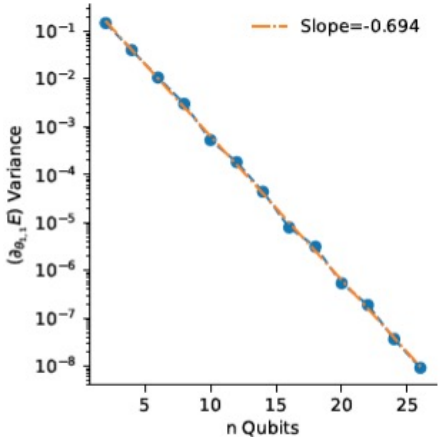
Model Convergence and Barren Plateau

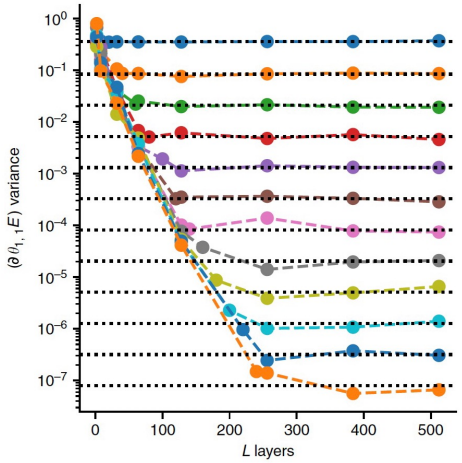
J. McClean et al., arXiv:1803.11173

Given the size of the Hilbert space a compromise between **expressivity**, **convergence** and **generalization** performance is needed.

Quantum gradient decay exponentially in the number of qubits

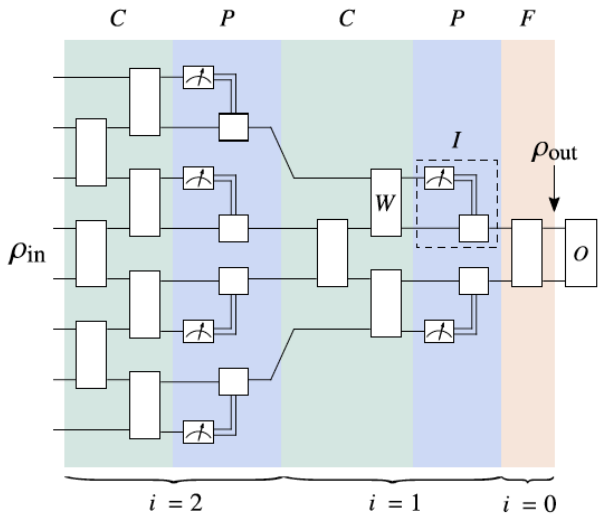
- Random circuit initialization
- Loss function locality in shallow circuits (M. Cerezo *et al.*, arXiv:2001.00550)
- Ansatz choice: TTN, CNN (Zhang *et al.*, arXiv:2011.06258, A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011.)
- Noise induced barren plateau (Wang, S *et al.*, Nat Commun 12, 6961 (2021))





QCNNs are resistant to barren plateaus due to their distance from low *T2-design* *(Pesah et al., arxiv:2011.02966)*

- variance of the gradient vanishes no faster than polynomially
- Pooling-based QCNN is trainable



QCNN: A Pesah, et al., Physical Review X 11.4 (2021): 041011

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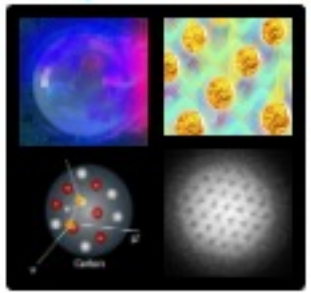
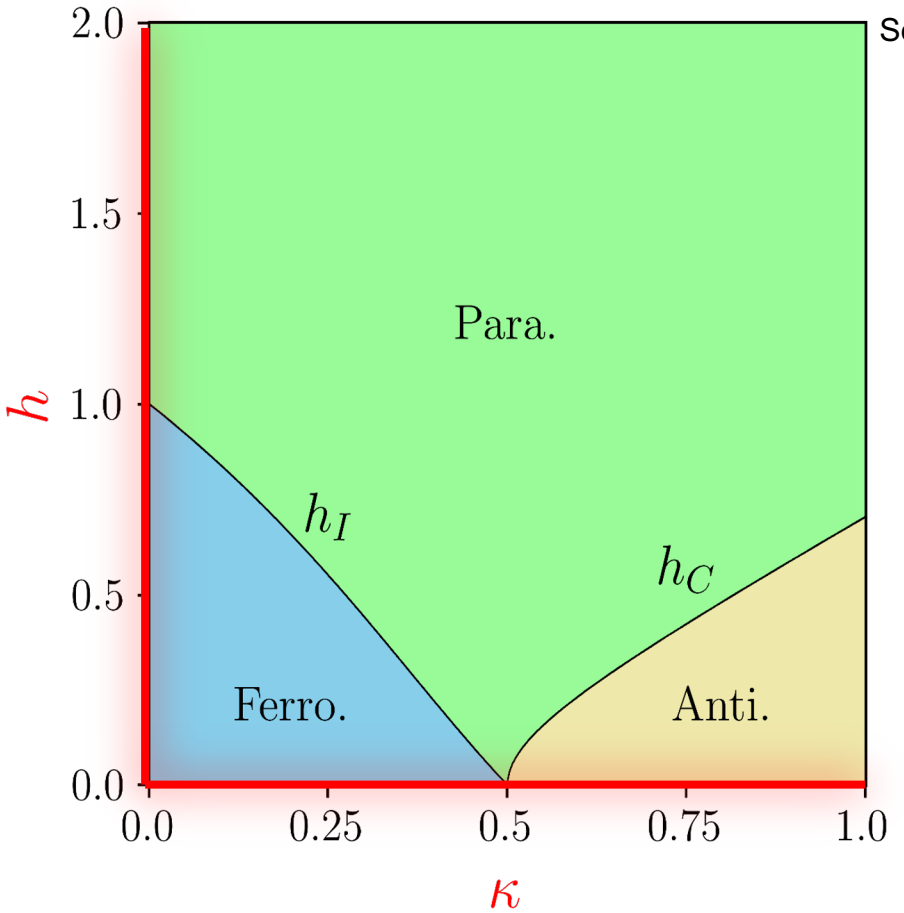


The Physics model: Axial Next Nearest Neighbor Ising (ANNNI)

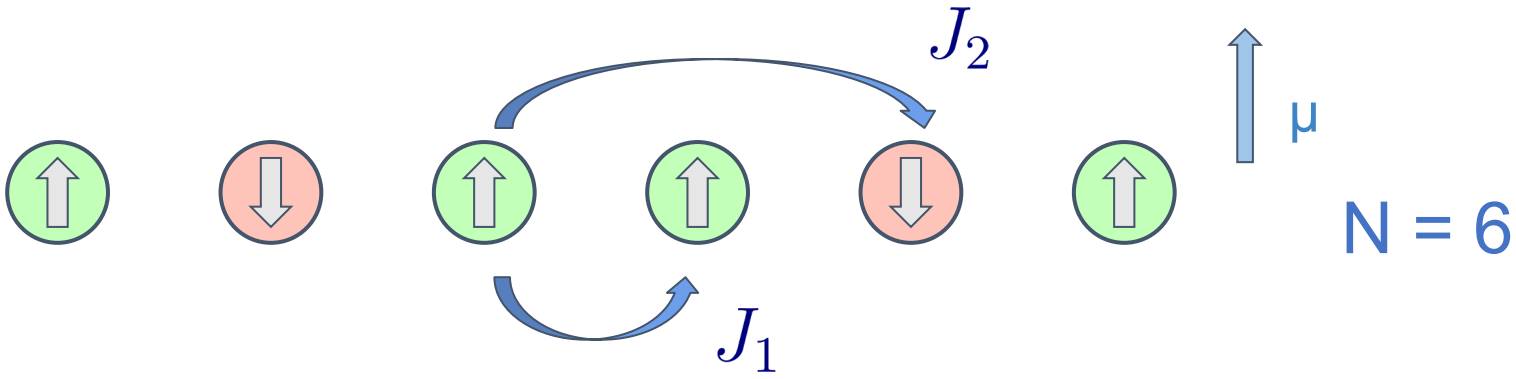
$$\mathcal{H} = -J_1 \sum_{i=1}^{N} \sigma_x^i \sigma_x^{i+1} - \kappa\, \sigma_x^i \sigma_x^{i+2} - h\, \sigma_z^i$$

$\kappa \equiv J_1/J_2$

$h \equiv \mu/J_1$



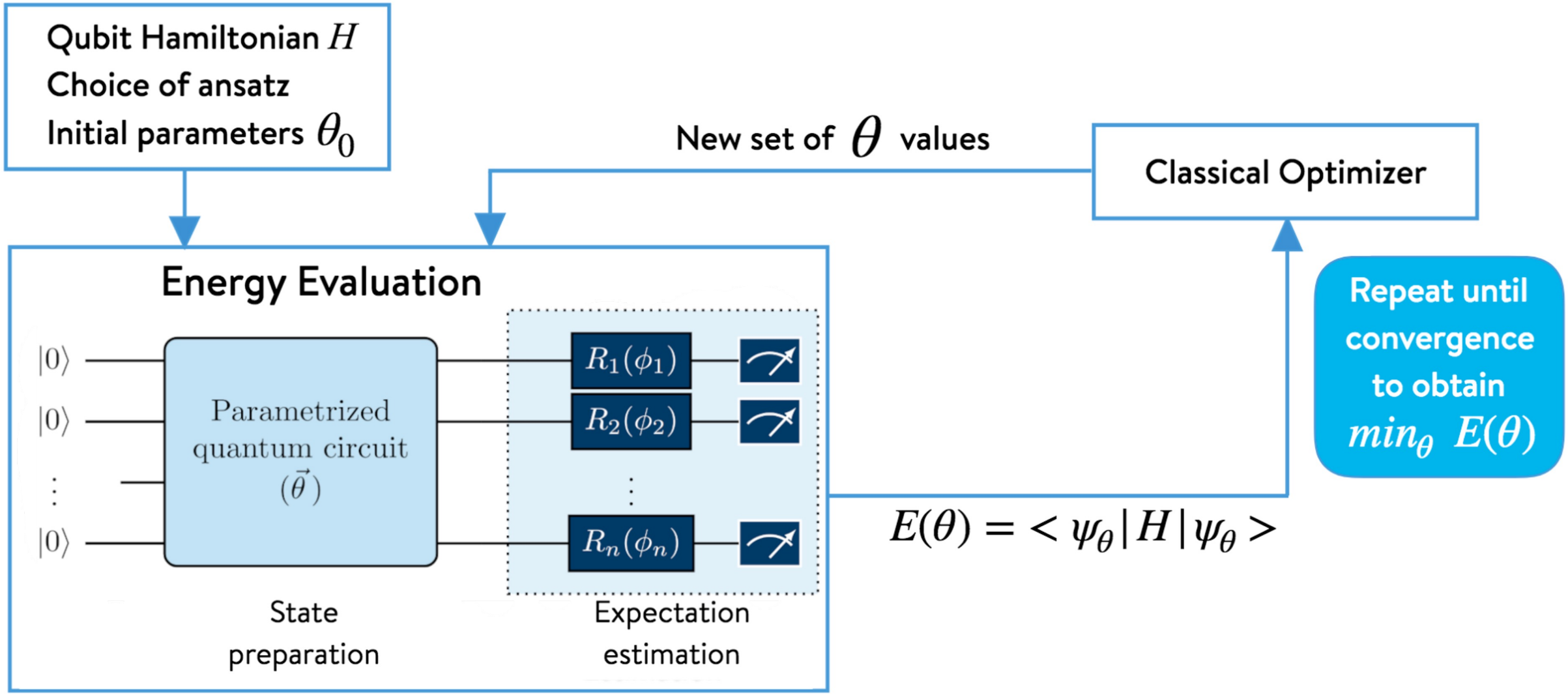
Senk, *Physics Reports*, **170**, 4 (1988)



Integrable only for:

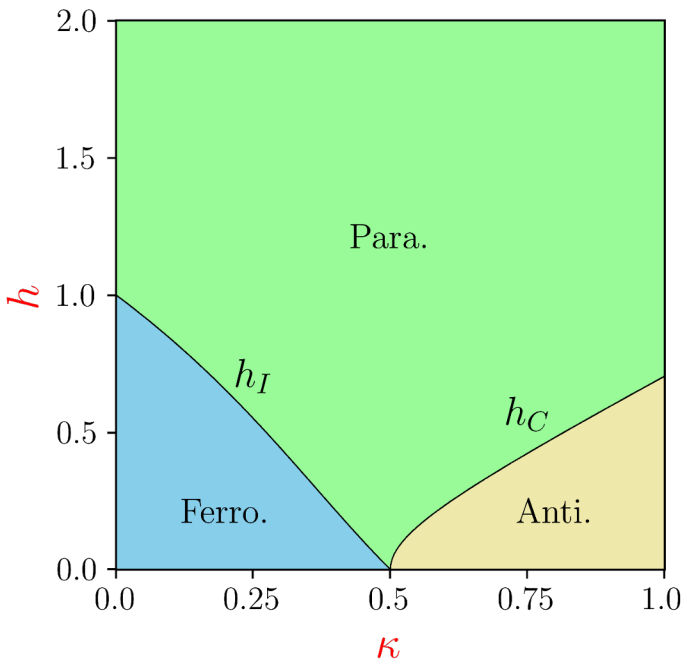
- $h = 0,\ \forall \kappa$ (x-axis)
- $\kappa = 0,\ \forall h$ (y-axis)

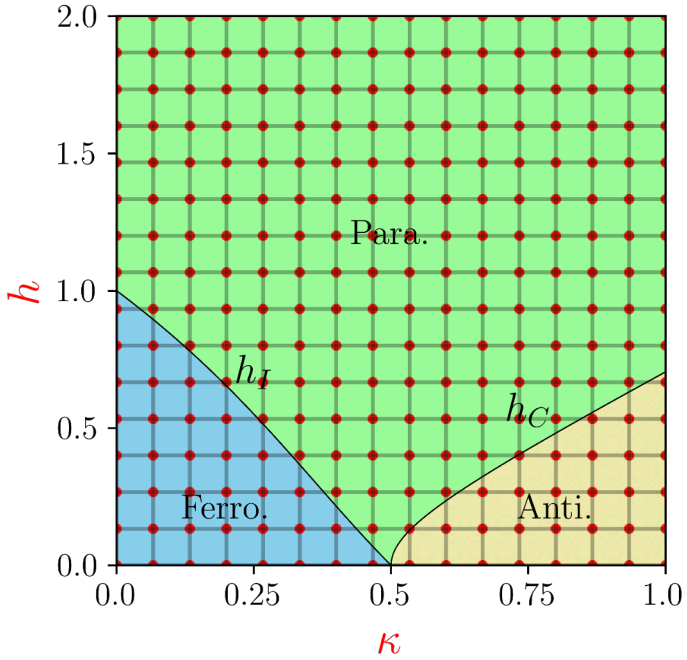
Variational Quantum Eigensolver (VQE)



Variational Quantum Eigensolver (VQE)

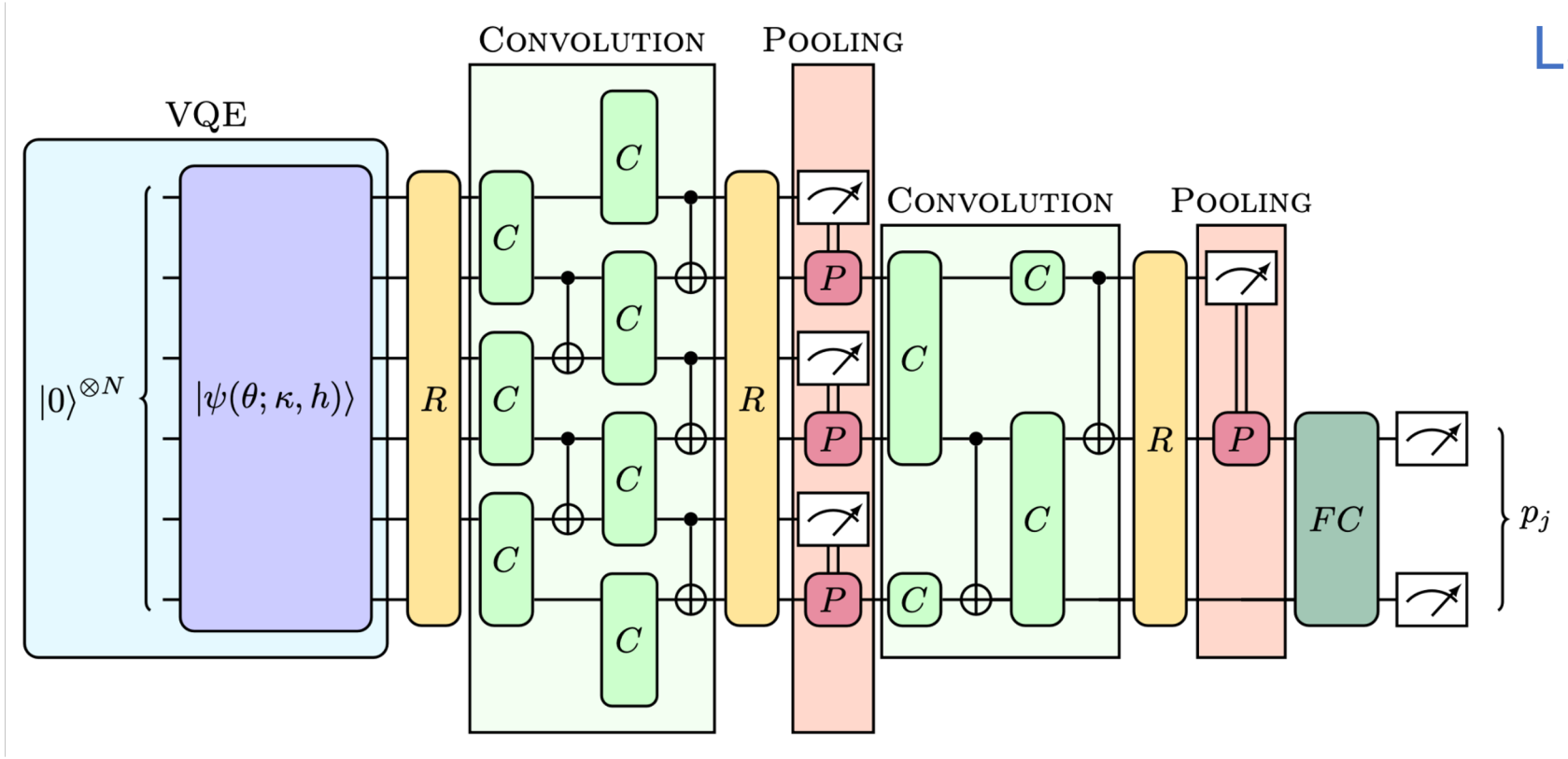
$$\mathcal{H}(\kappa, h) = -J_1 \sum_{i=1}^{N} \sigma_x^i \sigma_x^{i+1} - \kappa\, \sigma_x^i \sigma_x^{i+2} - h\, \sigma_z^i$$





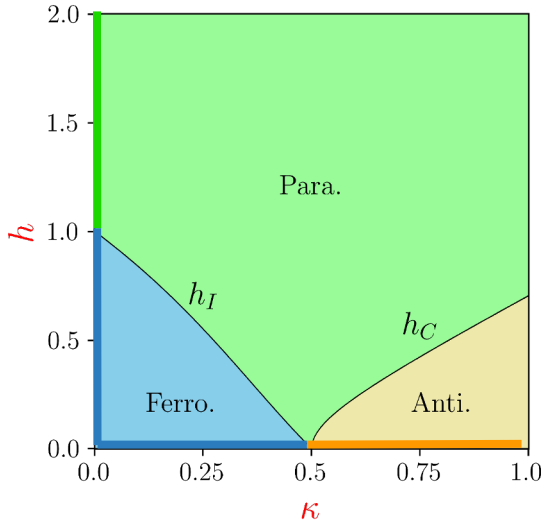
κ and h can assume 100 values each → 10,000 total states to obtain through VQE!

Quantum Convolutional Neural Network (QCNN)



Labels:

- [0,1] ferromagnetic
- [1,0] antiphase
- [1,1] paramagnetic
- [0,0] trash label



Binary Cross-entropy

Loss: $$\mathcal{L} = -\frac{1}{|\mathcal{S}_X^n|} \sum_{(\kappa,h)\in\mathcal{S}_X^n} \sum_{j=1}^{K} y_j(\kappa,h) \log\left(p_j(\kappa,h)\right)$$

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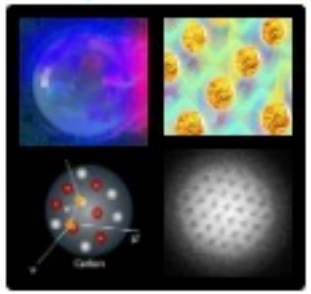
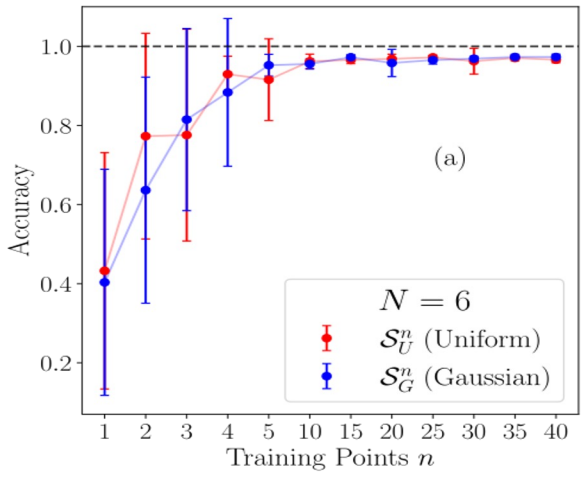
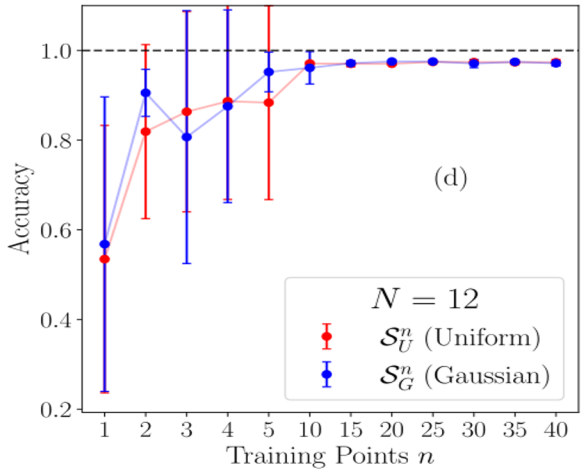


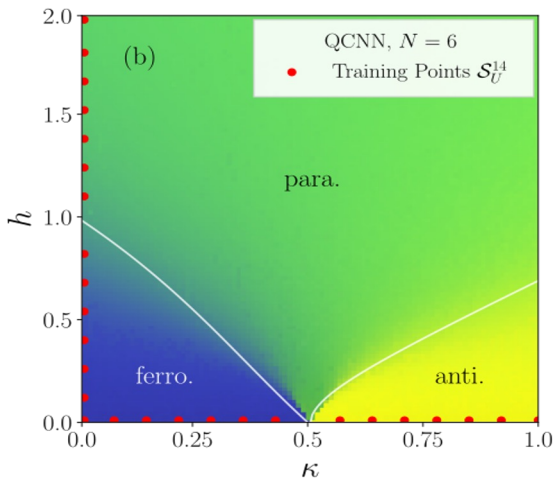
Results

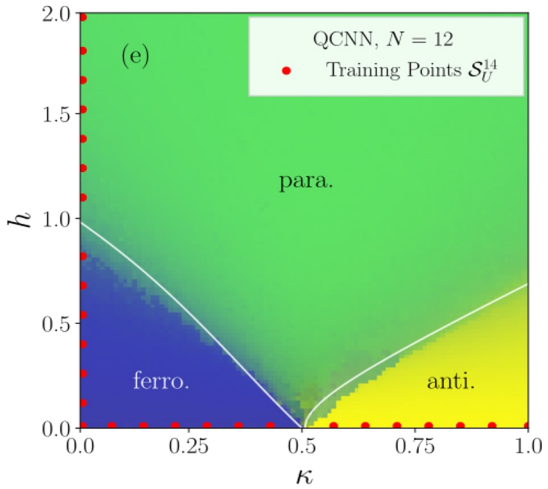
Training size

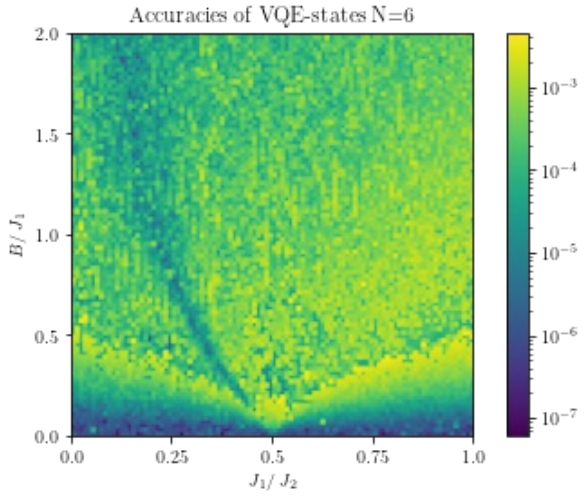




QCNN (95%)







- Normalised (exact diagonalisation – VQE)
- The accuracy is always above 99%.
- The *Peschel-Emery* line is exhibited, unravelling new physics by comparing VQE with different approaches, such as DMRG

Conclusion

1. QCNN trained (NO BP) on few training point for Quantum Phase Recognition
2. QCNN gives quantitative predictions

   [Banchi et all., Generalization in Quantum Machine Learning: A Quantum Information Standpoint, PRX QUANTUM 2, 040321 (2021)]
3. Performance increases with the system's size.
4. Adresses the bottleneck of needing expensive training labels
5. Potential Out of Distribution *Generalization*

   [M..Caro et al., Out-of-distribution generalization for learning quantum dynamics, https://arxiv.org/abs/2204.10268]

THANK YOU

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CERN Quantum Technology Initiative

Accelerating Quantum Technology Research and Applications

Paper

Code