

# Quantum phase detection generalisation from marginal quantum neural network models

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## Quantum Data through VQE

Ground-states of the ANNNI Hamiltonian

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

obtained through the Variational Quantum Eigensolver (VQE) [1]. The model is only trained on the **limiting integrable regions** where  $\kappa = 0$  (Ising) or  $h = 0$  (*quasi-classical*).

## Details on the QCNN

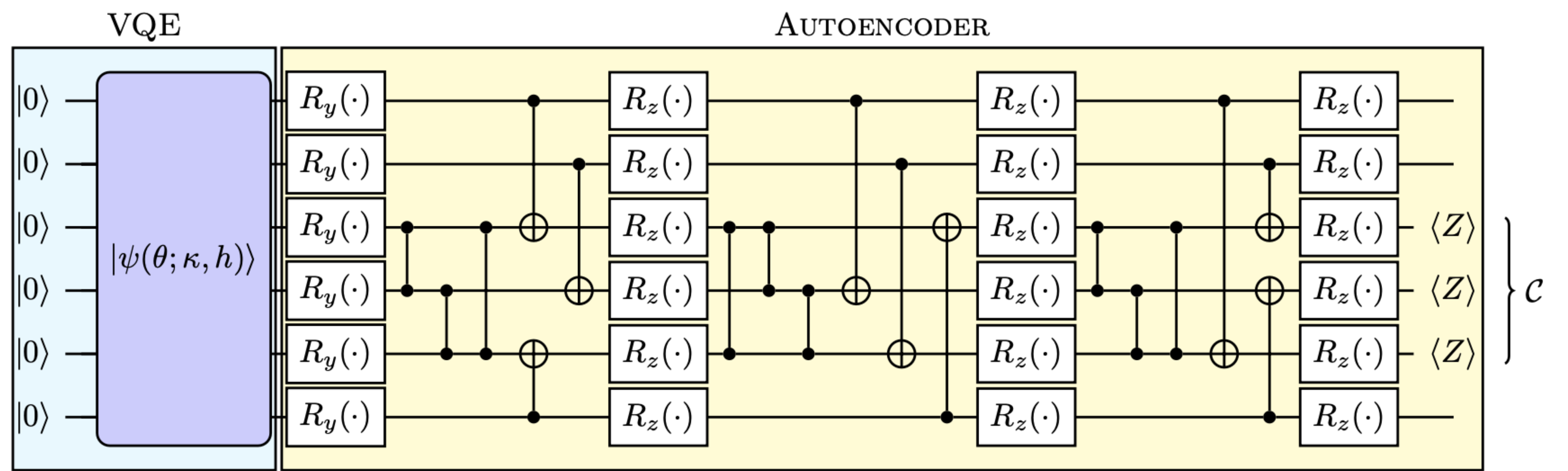
- **Supervised classifier.**
- Outputs the probability  $p_j$  to be in the  $j$ th phase (ferro-, para-magnetic or antiphase).
- Resistant to barren plateaus.
- Train with the cross entropy loss function

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

Gates (Repeat until there is two qubits left):

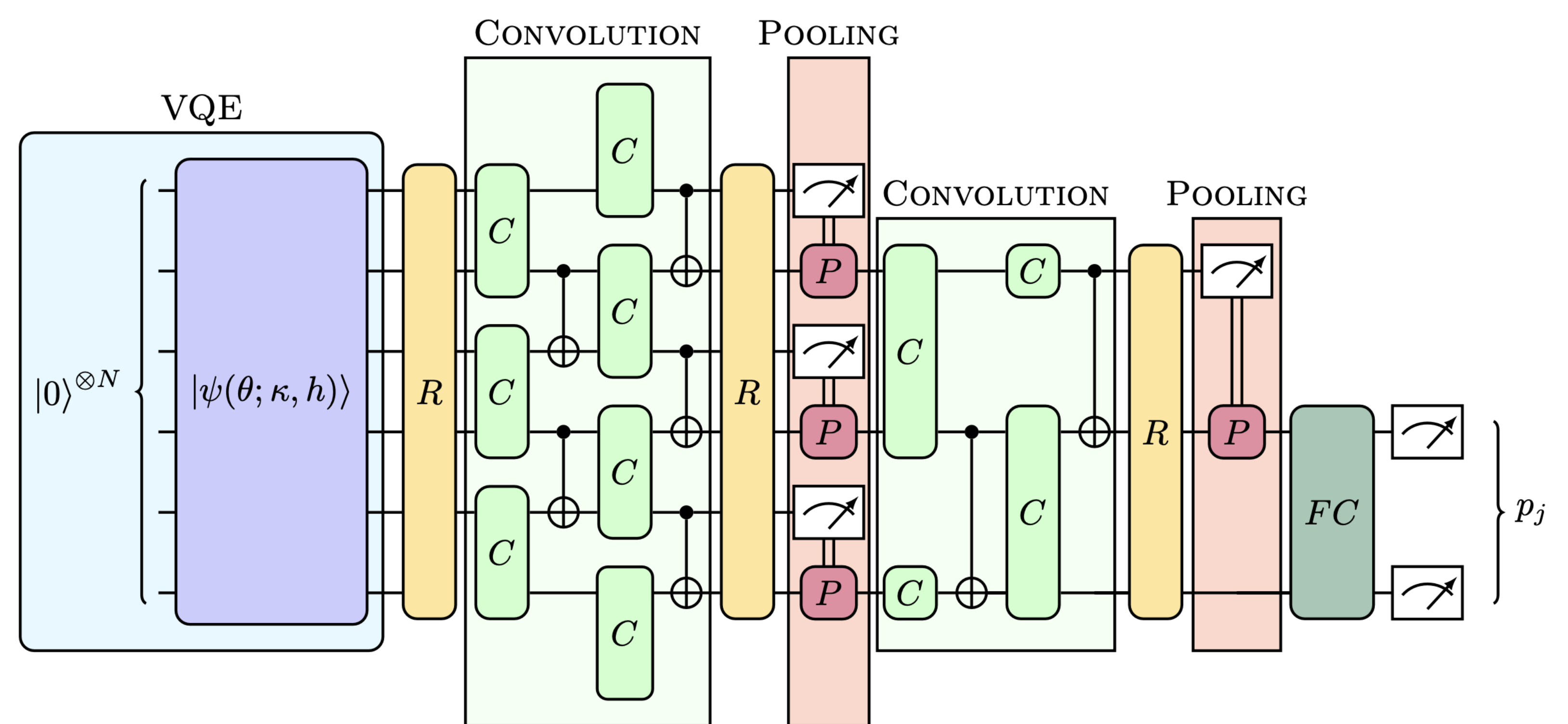
- **Free rotations:**  $R(\vec{\theta}) = \bigotimes_{i=1}^N R_y(\vec{\theta}_i)$ .
- **Two-qubit Convolutions:**  $C(\theta) = \bigotimes_{i=1}^2 R_y(\theta)$ .
- **Free rotations:**  $R(\vec{\theta}) = \bigotimes_{i=1}^N R_y(\vec{\theta}_i)$ .
- **Pooling:**  $P(\vec{\theta}, \phi, b) = R_y(\vec{\theta}_b) R_x(\phi)$  with  $b \in \{0, 1\}$  the value of the measured qubit.
- **Two-qubit fully connected:**  $F(\vec{\theta}^{(1)}, \vec{\theta}^{(2)}) = \left( \bigotimes_{i=1}^2 R_y(\vec{\theta}_1^{(i)}) R_x(\vec{\theta}_2^{(i)}) R_y(\vec{\theta}_3^{(i)}) \right) CX_{1,2}$ .

## Anomaly Detection with a Quantum Autoencoder [2]



(Unsupervised technique) The autoencoder compresses the initial state and assign an anomaly score  $\mathcal{C} = \frac{1}{2} \sum_{j \in q_T} (1 - \langle Z_j \rangle)$  to each point in the phase diagram.

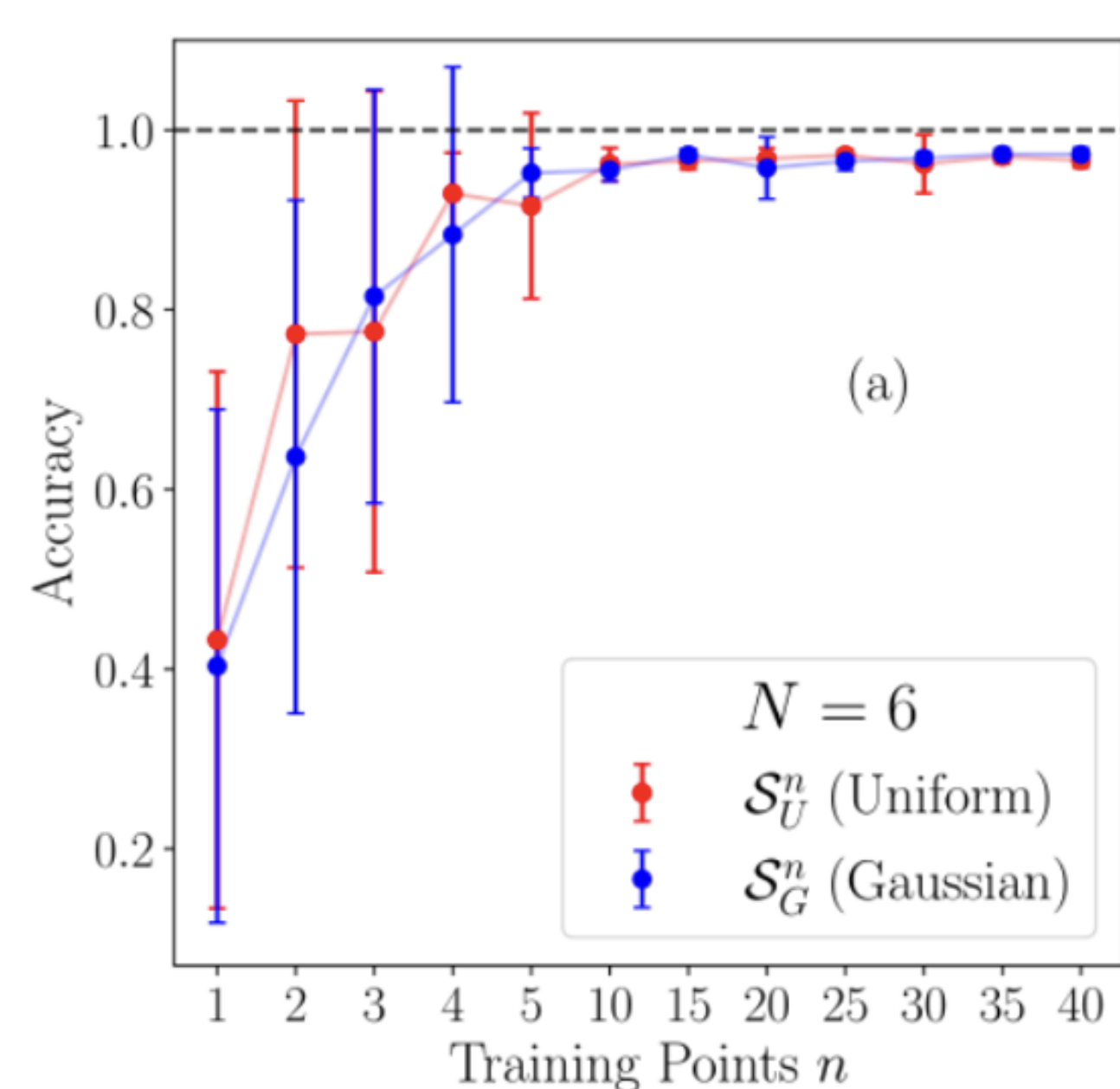
## Quantum Convolutional Neural Network (QCNN) [3]



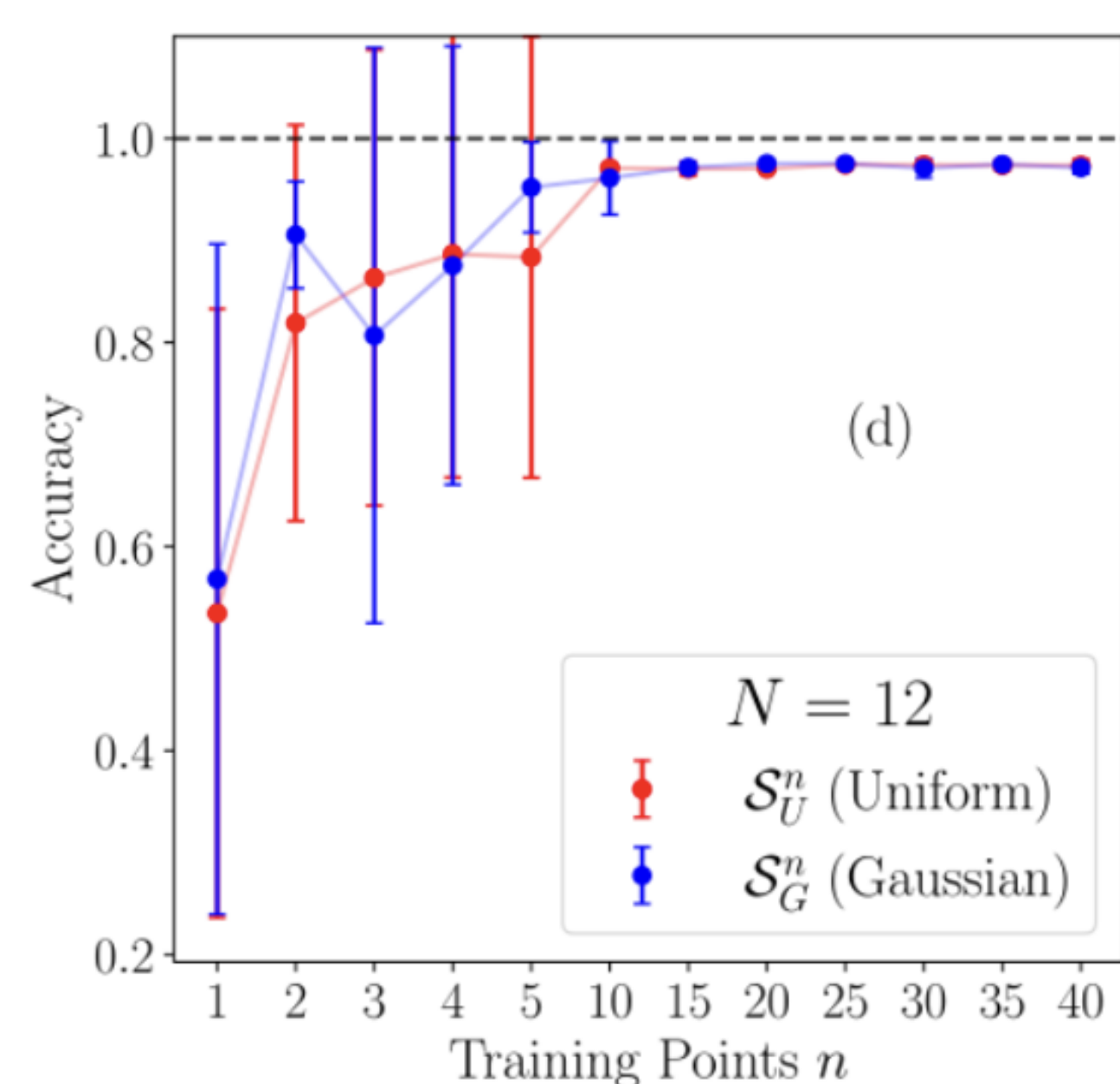
## Generalisation from training on the boundaries [5]:

### Size of training set

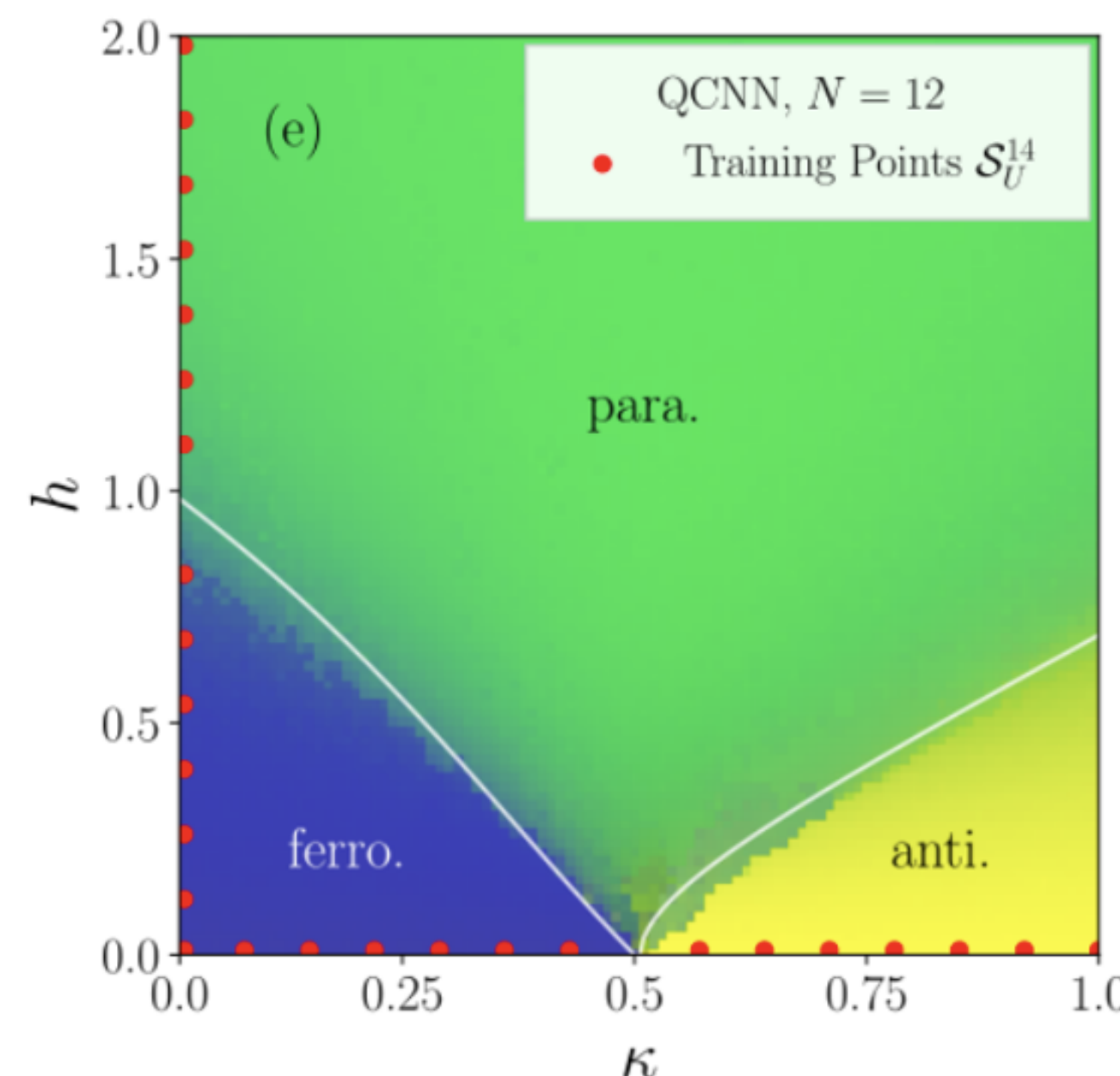
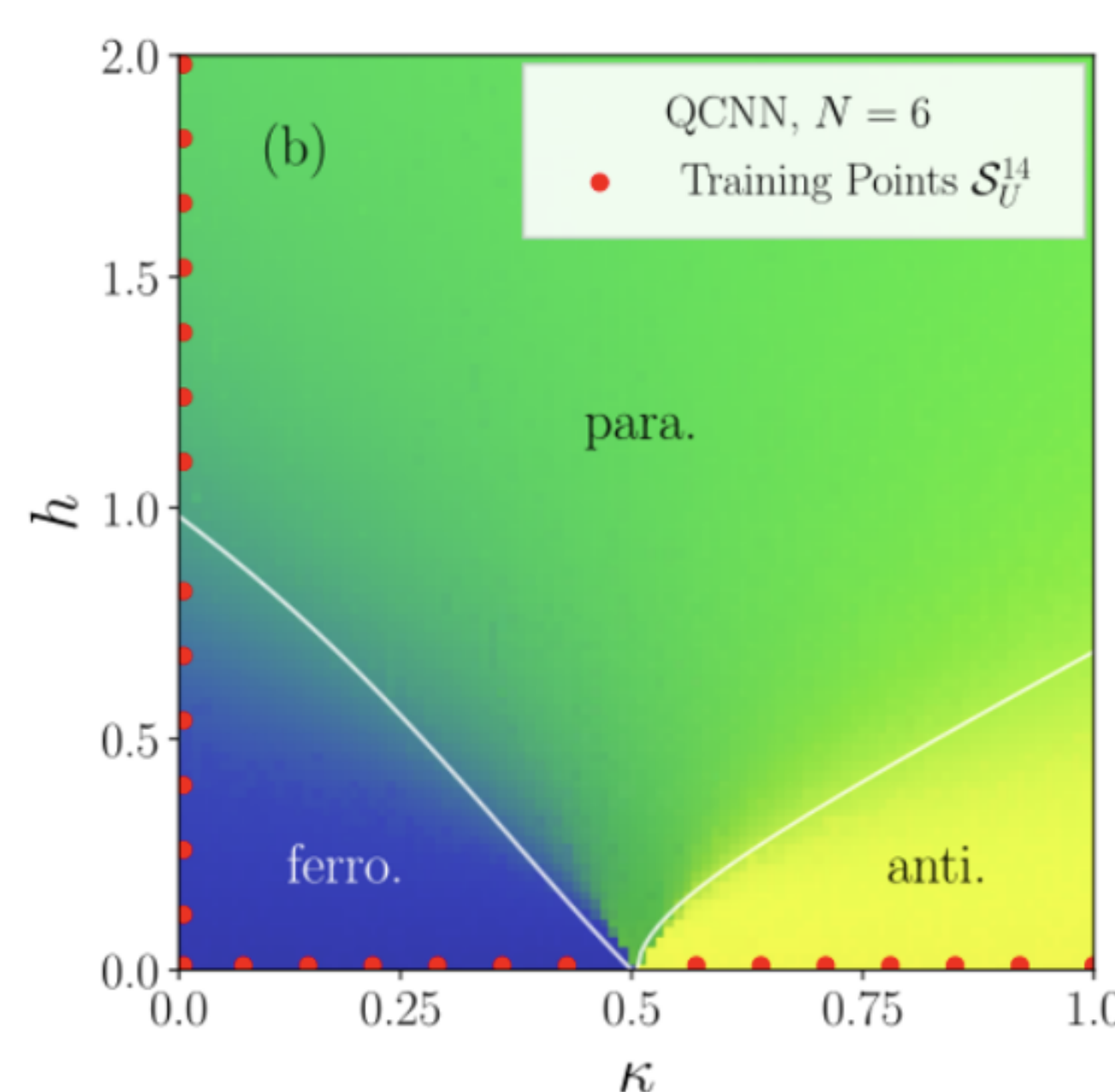
$N = 6$



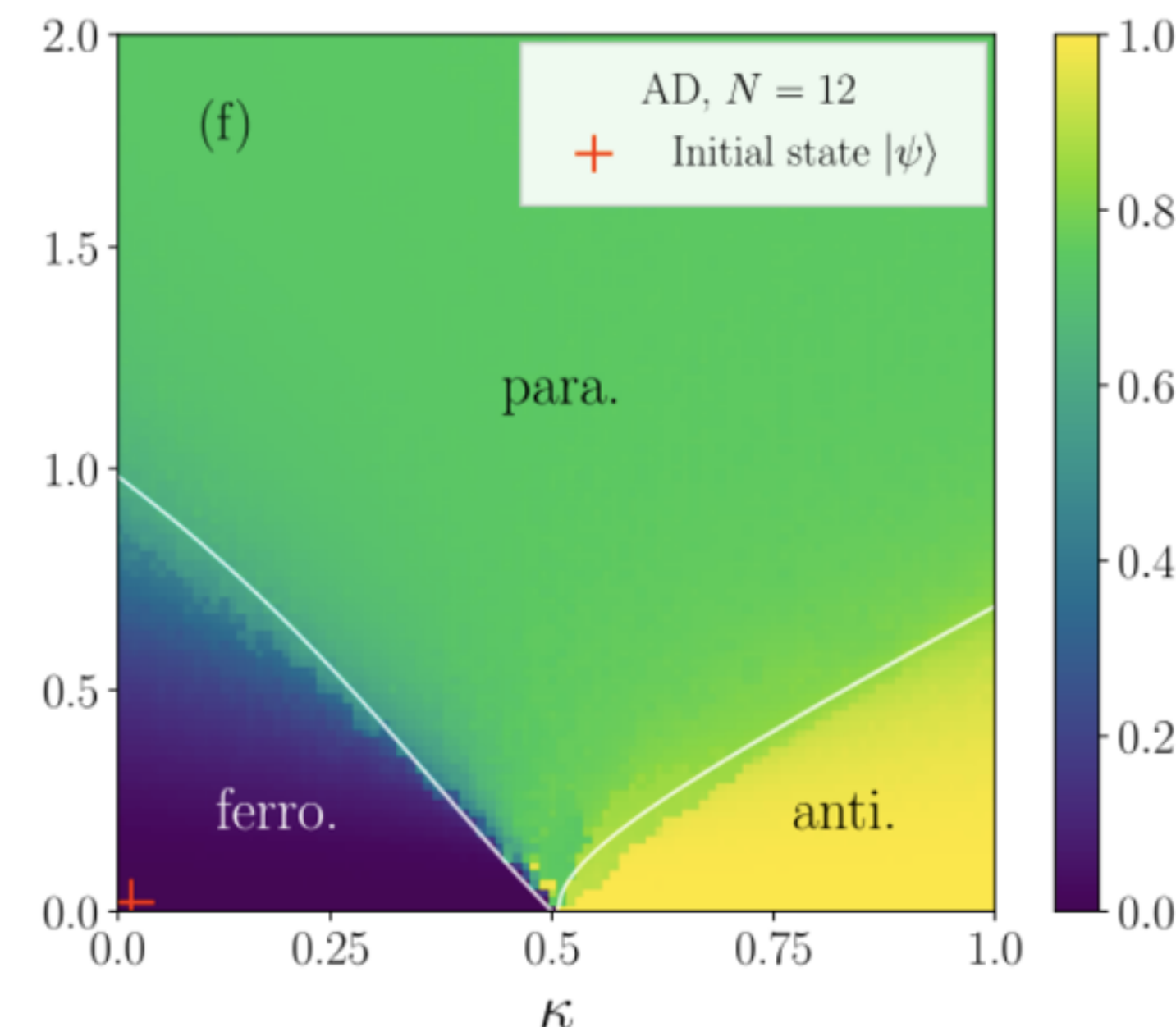
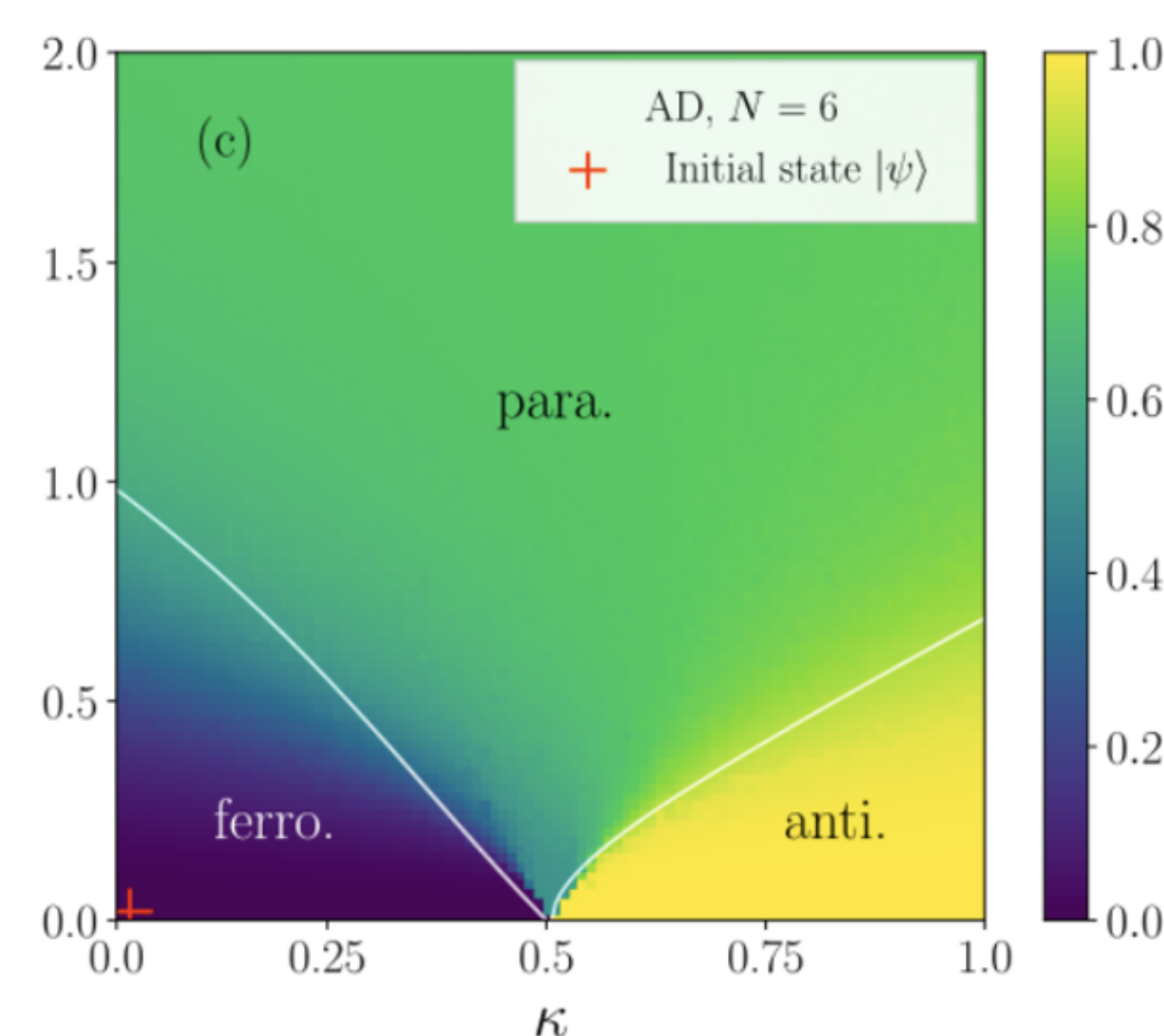
$N = 12$



### QCNN



### Autoencoder



### Conclusions

- Generalisation from few training points [4].
- Performance increases with the system's size.
- Addresses the bottleneck of needing expensive training labels.

## References

- [1] Peruzzo, A. et al., *Variational eigenvalue solver on a photonic quantum processor*, Nat. Commun. **5**, 4123 (2014).
- [2] Kottmann, K. et al, *Variational quantum anomaly detection: Unsupervised mapping of phase diagrams on a physical quantum computer*, Phys. Rev. Research **3**, 043184 (2021)
- [3] Cong, I., Choi, S. and Lukin, M.D. *Quantum convolutional neural networks*, Nat. Phys. **15**, 1273–1278 (2019)
- [4] Caro, M. et al, *Generalization in quantum machine learning from few training data*, Nat Commun **13**, 4919 (2022)
- [5] Monaco, S. et al, *Quantum phase detection generalisation from marginal quantum neural network models*, ArXiv: 2208.08748 (2022)