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

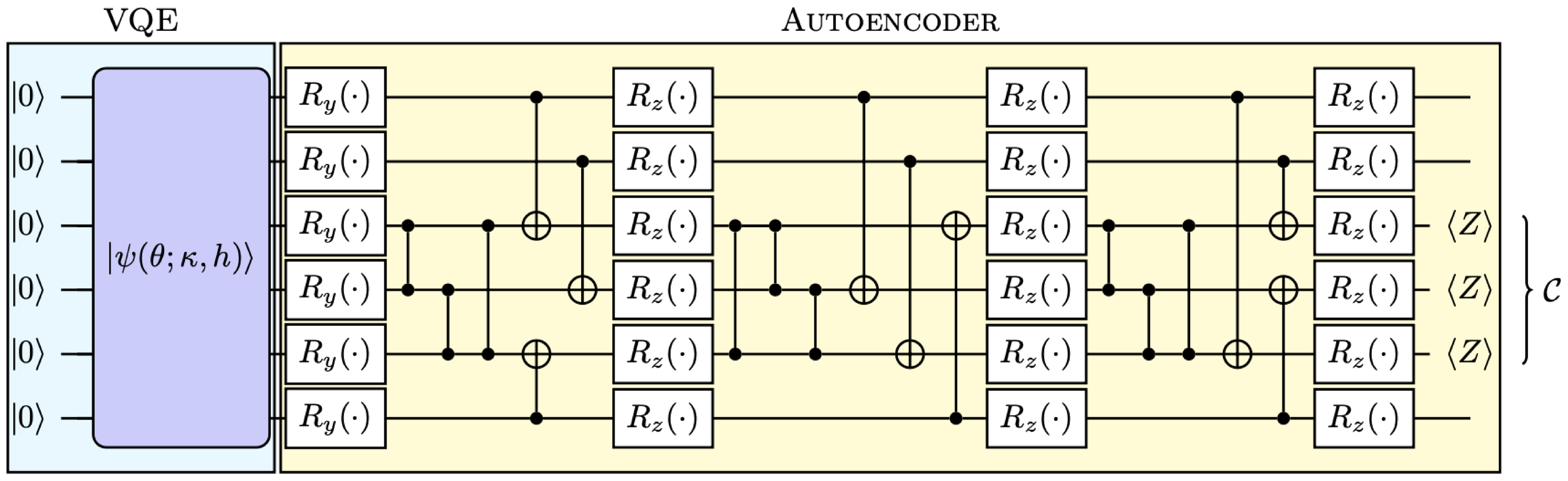
- **Supervised classifier.**
- Outputs the probability p_j to be in the jth phase (ferro-, para-magnetic or antiphase).
- Resistant to barren plateaus.
- Train with the cross entropy loss function

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

Gates (Repeat until there is two qubits left):

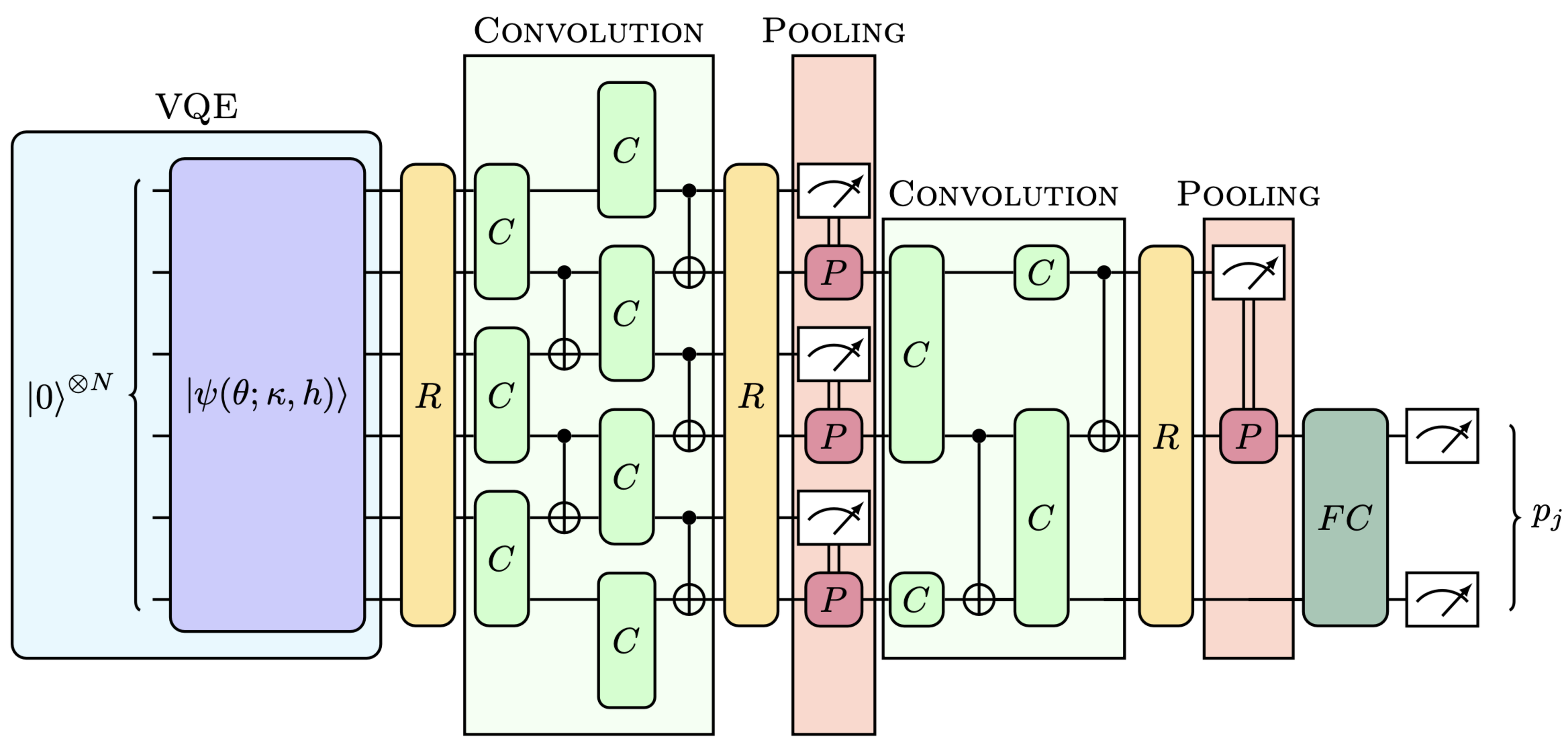
- Free rotations: $R(\vec{\theta}) = \bigotimes_{i=1}^{N} R_y(\vec{\theta}_i)$.
- Two-qubit Convolutions: $C(\theta) = \bigotimes_{i=1}^{2} R_y(\theta)$.
- Free rotations: $R(\vec{\theta}) = \bigotimes_{i=1}^{N} R_y(\vec{\theta}_i)$.
- Pooling: $P(\vec{\theta}, \phi, b) = R_y(\vec{\theta}_b) R_x(\phi)$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

Anomaly Detection with a Quantum Autoencoder [2]

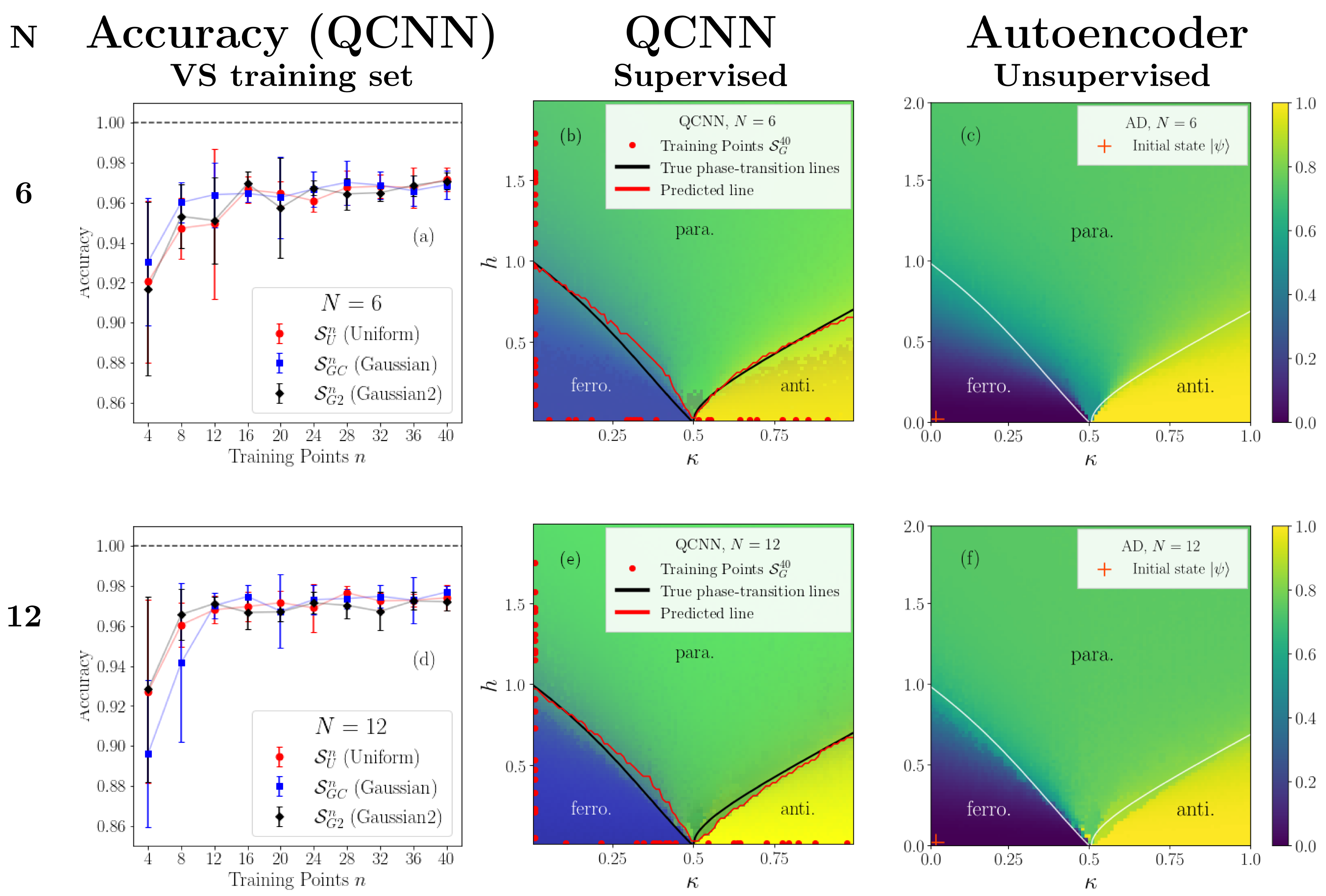


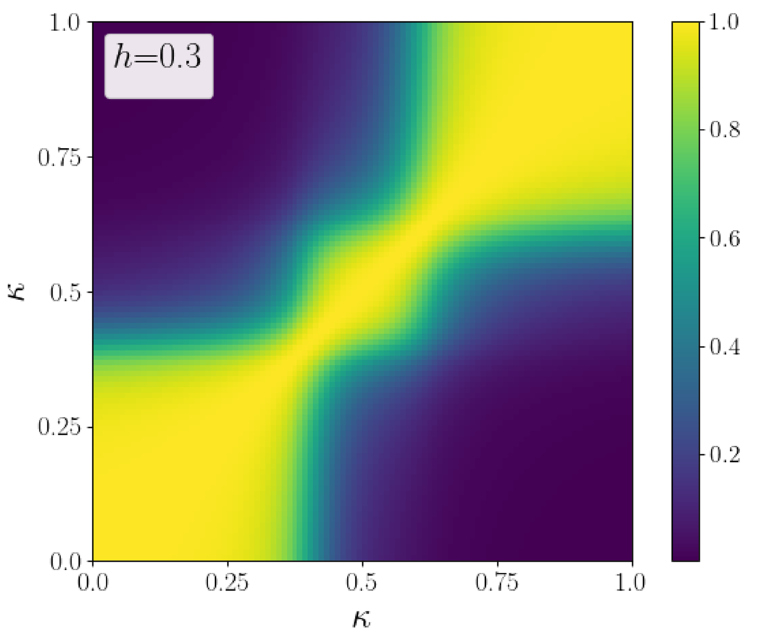
(Unsupervised technique) The autoencoder compresses the initial state and assign an anomaly score $\mathcal{C} = \frac{1}{2}\sum_{j\in q_T}(1 - \langle Z_j\rangle)$ to each point in the phase diagram.

Quantum Convolutional Neural Network (QCNN) [3]



Generalisation from training on the boundaries [5]:





Fidelity: $|\langle\psi(\kappa_i, h=0.3)|\psi(\kappa_j, h=0.3)\rangle|^2$.

Conclusions

- States are clustered.
- Out-of-distribution generalization from few training points [4].
- Addresses the bottleneck of expensive training labels.

References

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Resources

Code

Paper