Exploiting symmetry in variational quantum machine learning

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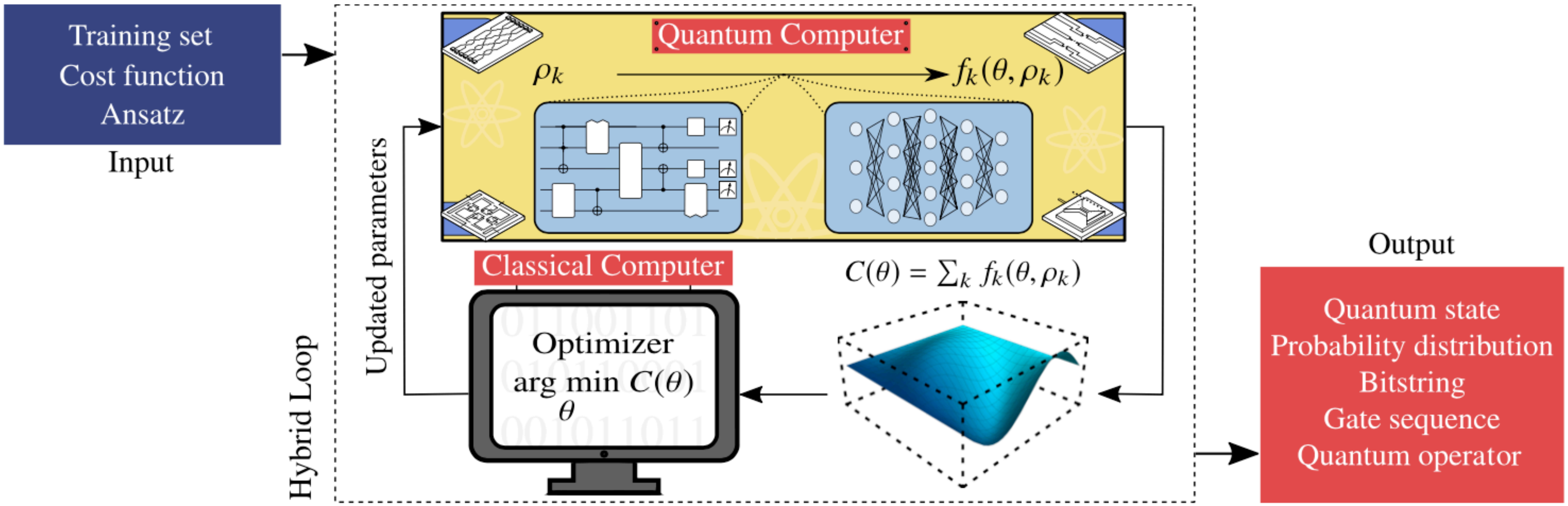
Variational Quantum Algorithms

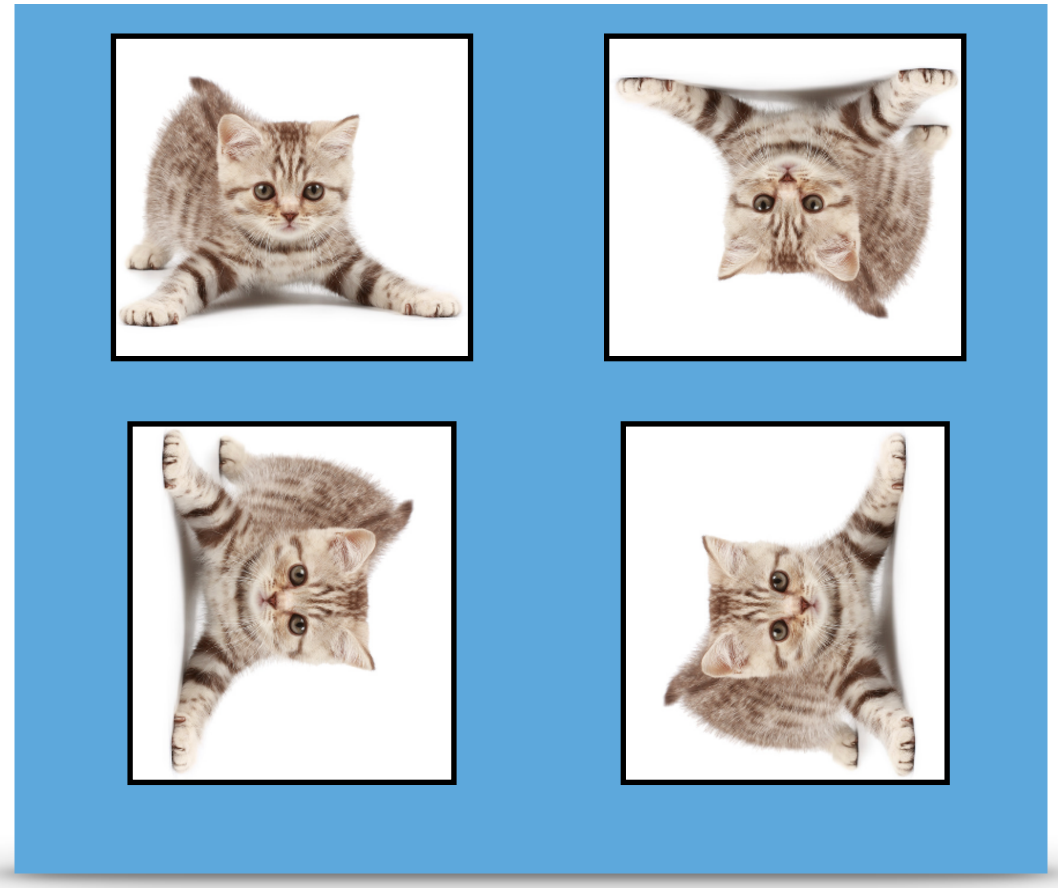


Marco Cerezo et al., Nature Reviews Physics (2021)

Commonly used for:

- **Machine Learning**
- **Quantum many-body problems**

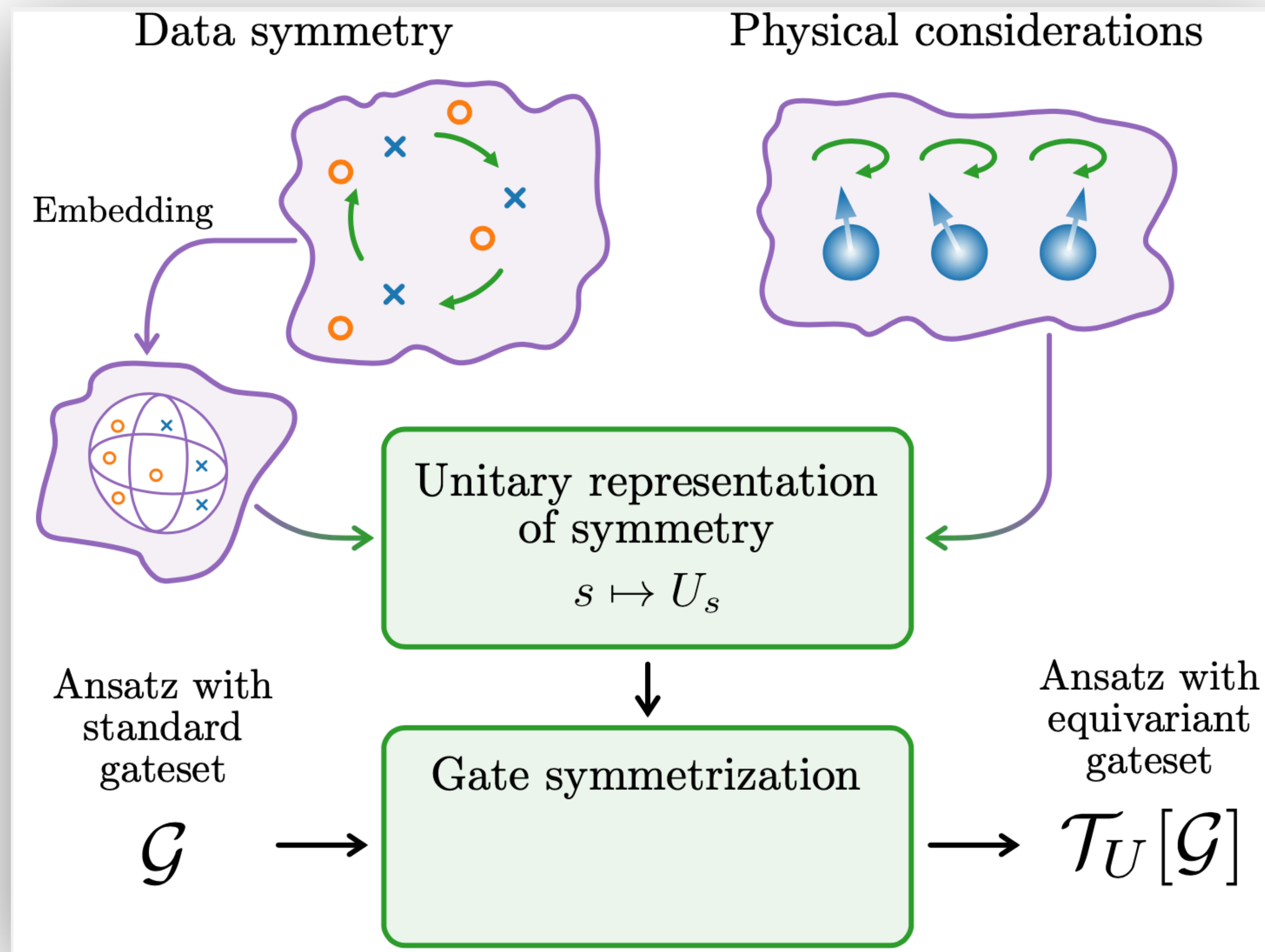
→ **Problems with Exploitable symmetries**



No matter how you turn the picture, it depicts always a cat!

Bronstein et al., ArXiv (2021)

Geometric Deep Learning



Make your learning model symmetry-aware

GOAL: Build invariant QML model

Symmetry invariant: $y(V_s[\boldsymbol{x}]) = y(\boldsymbol{x})$ where $y(\boldsymbol{x}) = \langle \psi(\boldsymbol{\theta}, \boldsymbol{x}) | O | \psi(\boldsymbol{\theta}, \boldsymbol{x}) \rangle$

V_s symmetry transformation on the data

We consider: $|\psi(\boldsymbol{\theta}, \boldsymbol{x})\rangle = W_L(\boldsymbol{\theta})U(\boldsymbol{x})\ldots W_1(\boldsymbol{\theta})U(\boldsymbol{x})W_0(\boldsymbol{\theta})|\psi_0\rangle$
where $U(\boldsymbol{x})$ is ***"equivariant"*** iff $U(V_s[\boldsymbol{x}]) = U_s U(\boldsymbol{x}) U_s^\dagger$

- $[U_s, W_l(\boldsymbol{\theta})] = 0$ ★
- $[U_s, O] = 0$
- $U_s |\psi_0\rangle = |\psi_0\rangle$

→ Symmetry invariant model

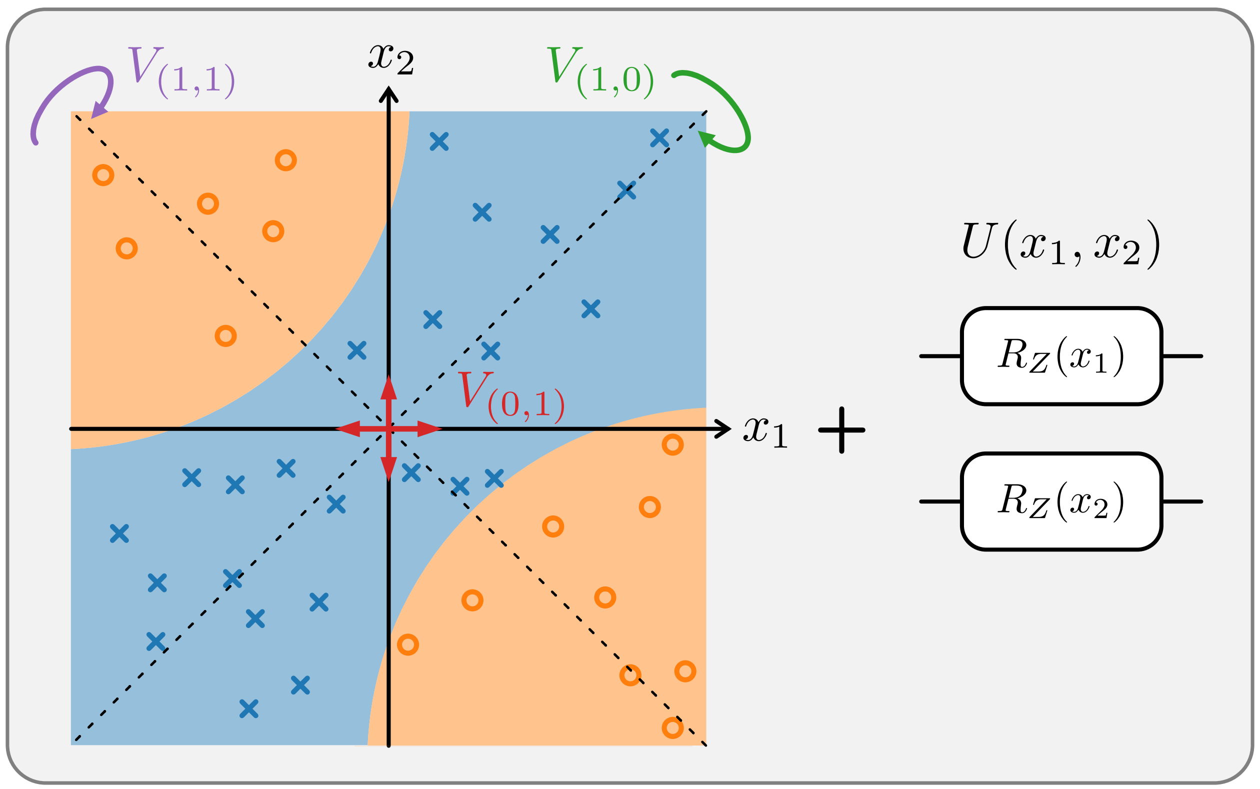
The "Twirling formula" $\mathcal{T}_U[X] = \frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} U_s X U_s^\dagger$ helps to satisfy ★

$W_l(\boldsymbol{\theta}) = \exp(-i\theta_l X)$

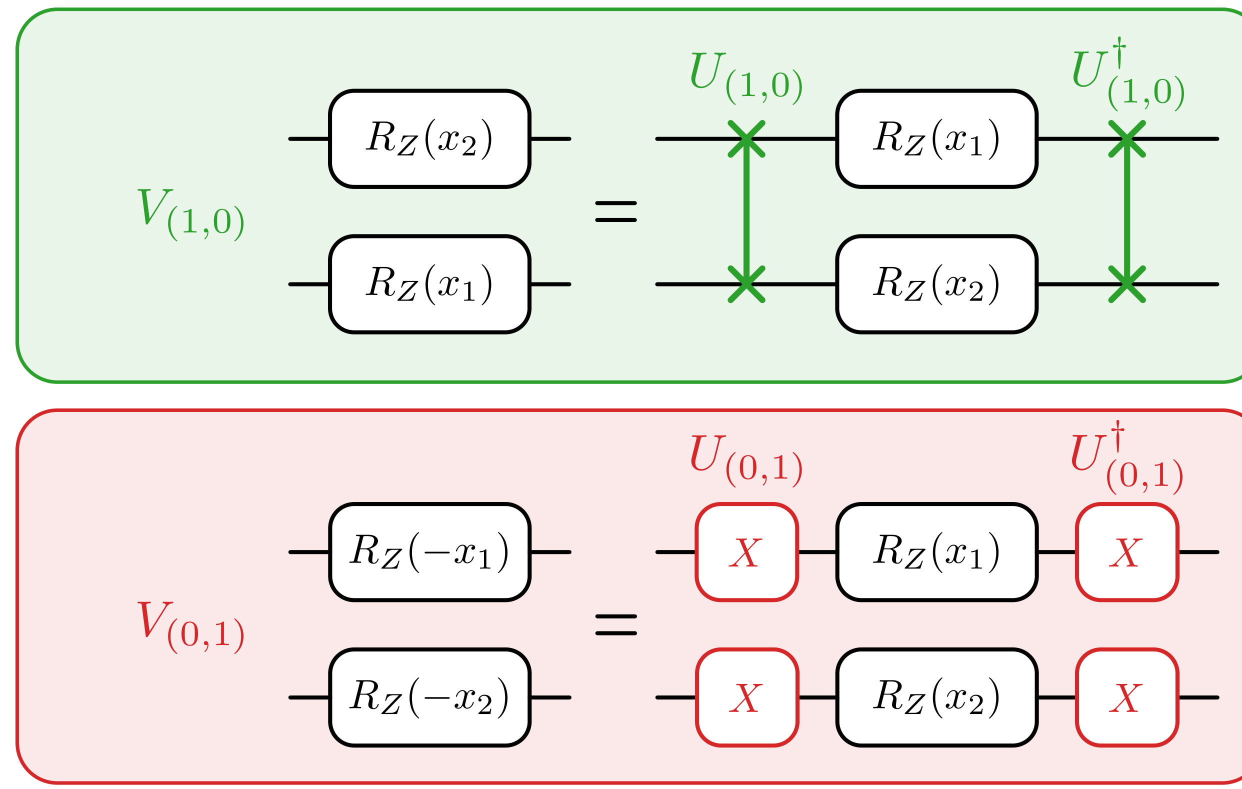
Equivariant embedding example

Dataset with features (x_1, x_2) :

$$y(x_1, x_2) = y(x_2, x_1) = y(-x_1, -x_2)$$



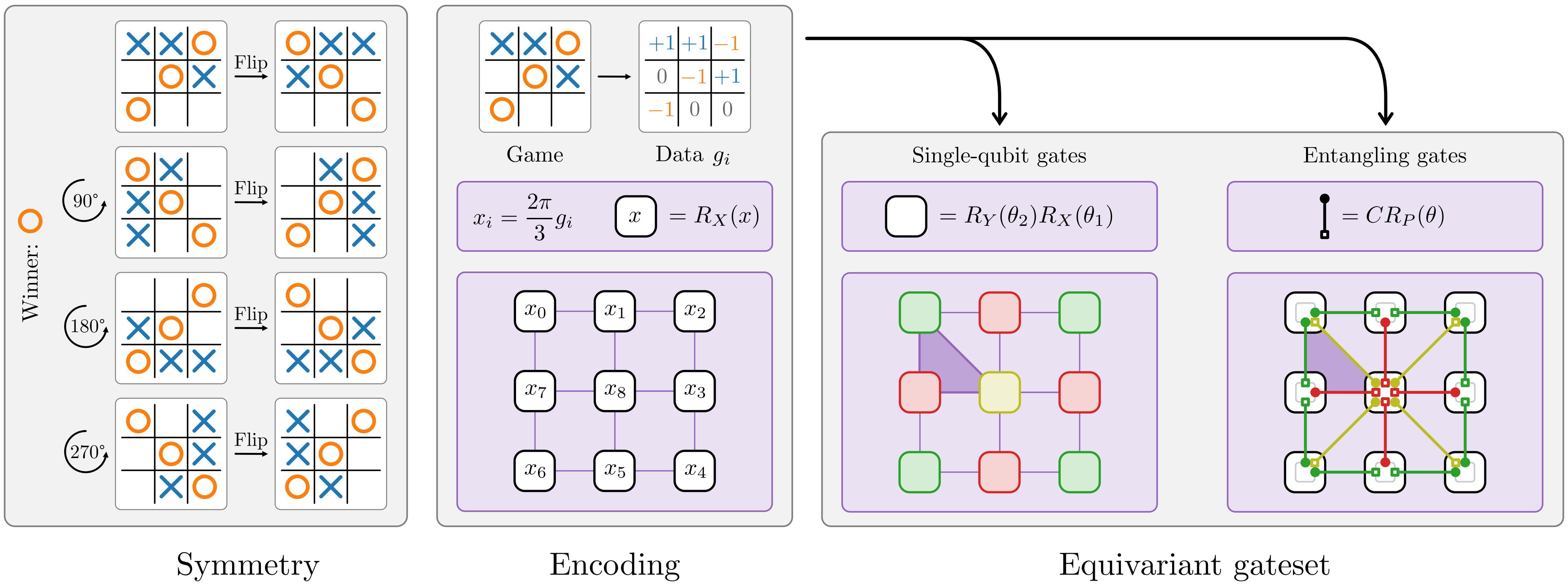
$\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric problem + Embedding

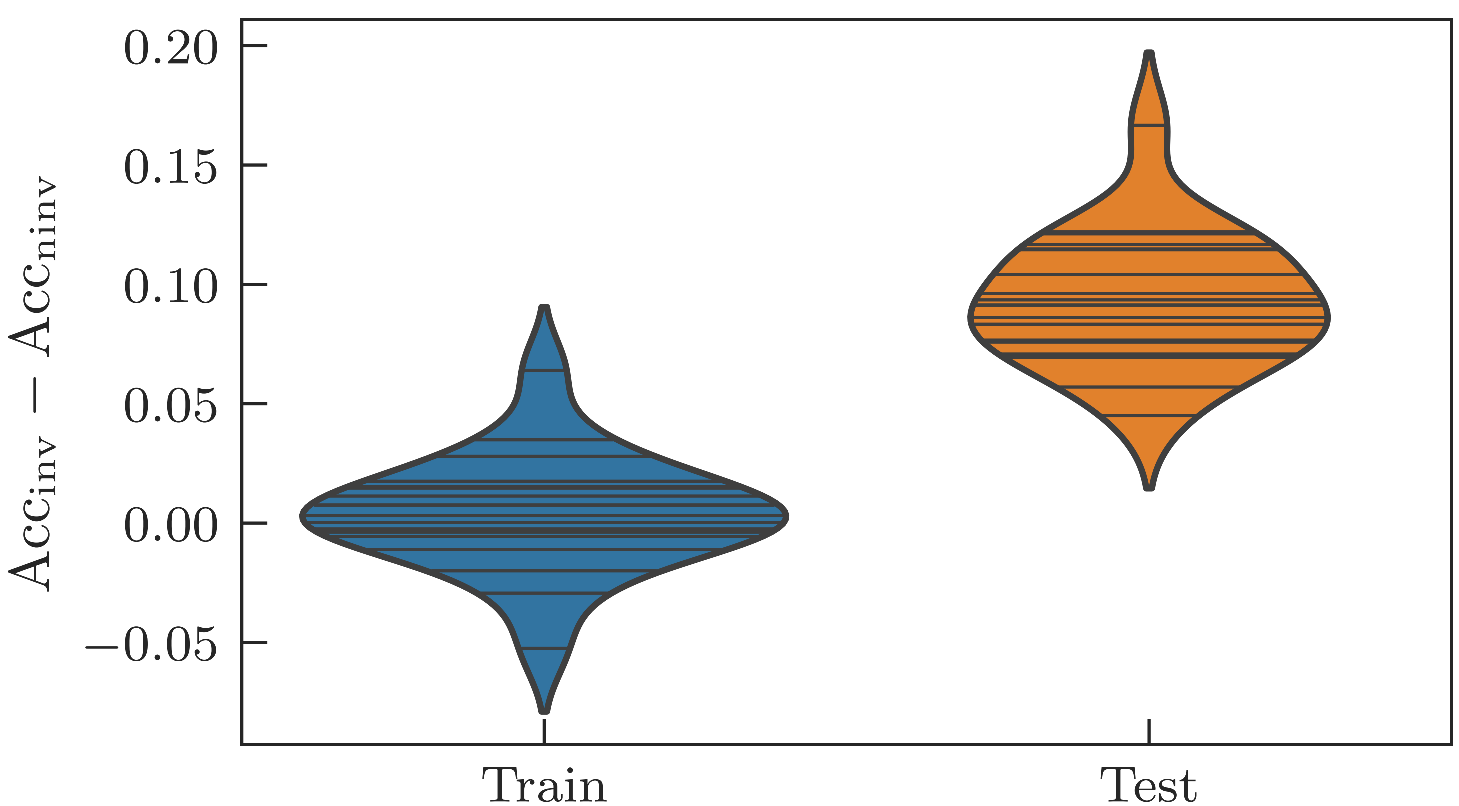


Induced representation

Symmetry operations on the data → Unitary transformations on the underlying Hilbert space

Numerical simulations: TIC-TAC-TOE





- **Similar performance on training**
- **But better on test for the invariant model**

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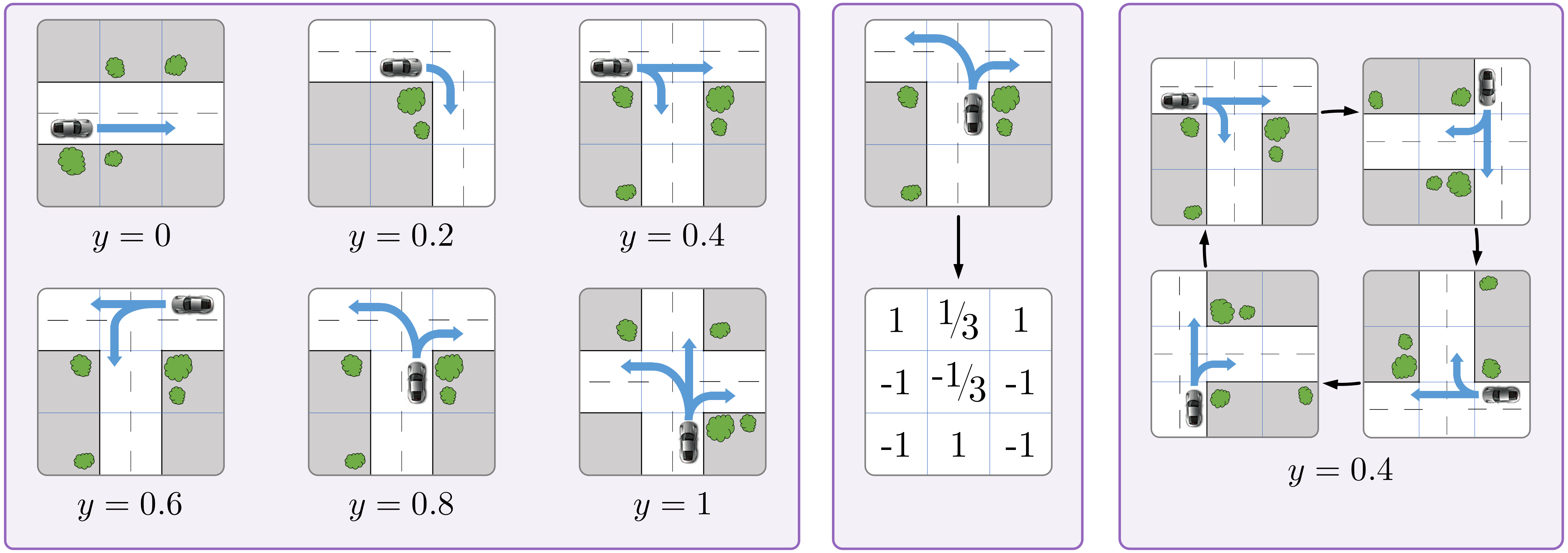
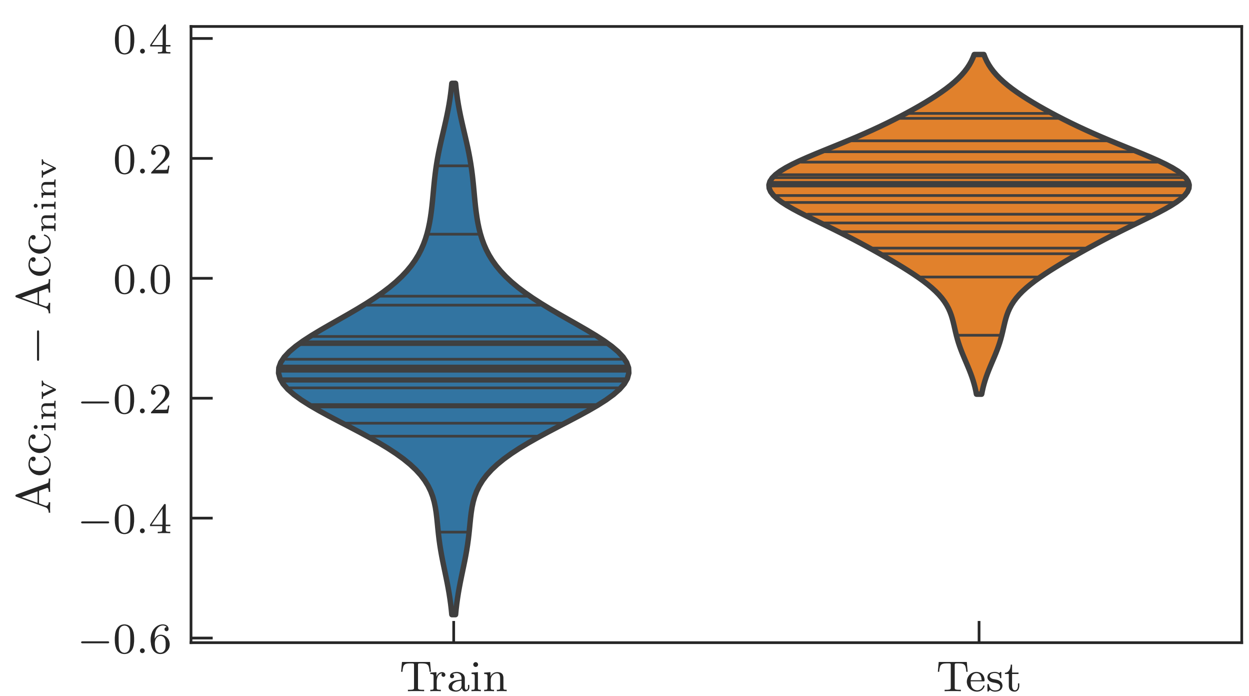
AUTONOMOUS CAR



Examples of difficulties Representation Symmetry



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Variational Quantum Eigensolver

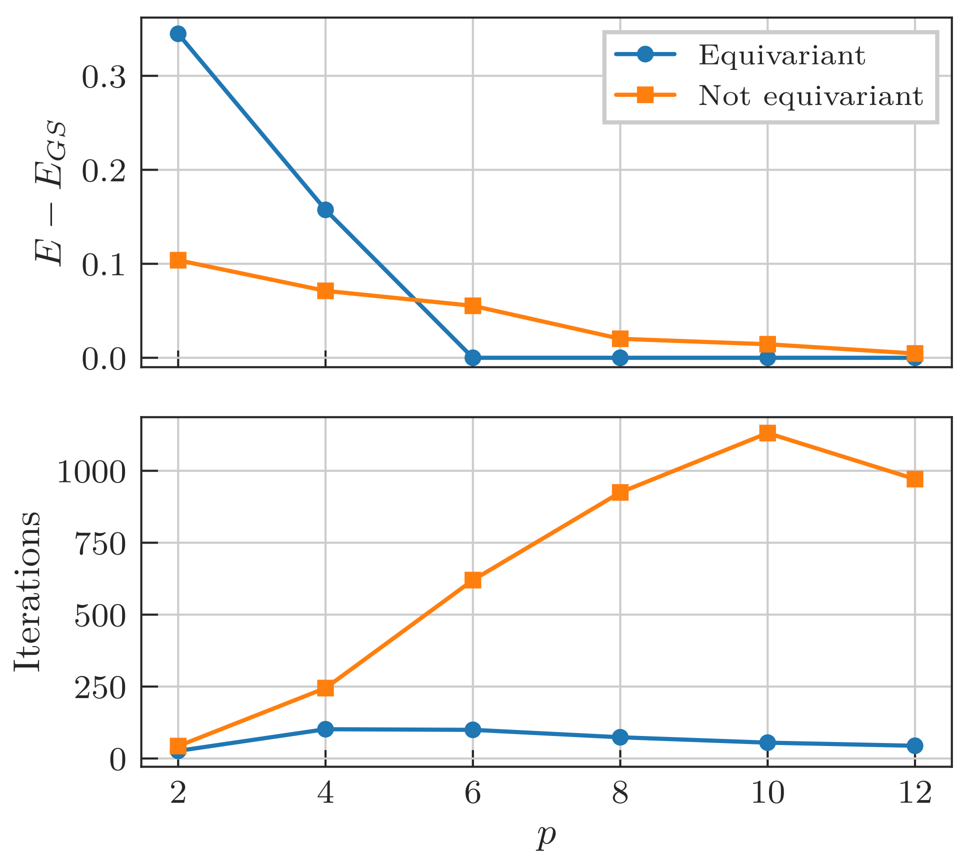
$$H_{TFIM} = -\sum_{i=1}^{N} Z_i Z_{i+1} - g \sum_{i=1}^{N} X_i$$

Spin-flip symmetry: $\left[\mathrm{P}, H_{TFIM}\right] = 0$ with $\mathrm{P} = \prod_{i=1}^{N} X_i$

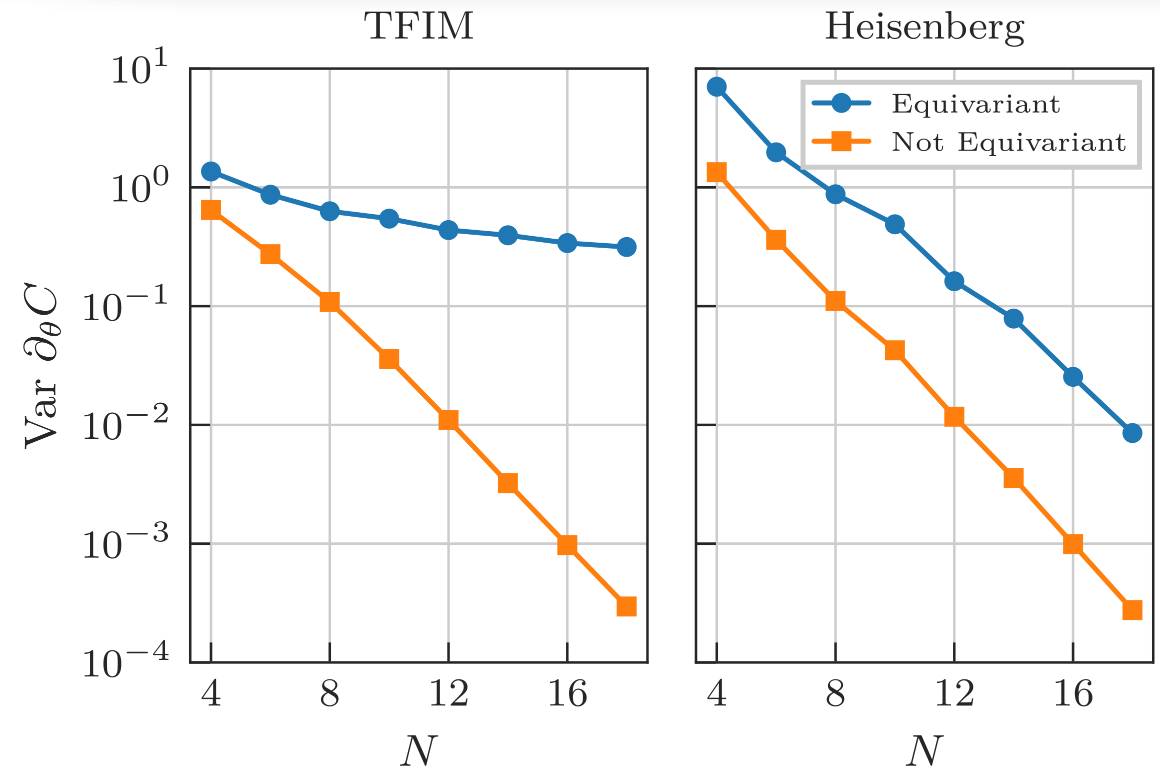
Extension of the equivariant construction to VQE:

$$|\psi(\alpha,\beta,\gamma)\rangle = \prod_{m=1}^{p} \boxed{\cancel{\prod_{i=1}^{N} e^{-i\alpha_m Y_i}}} \prod_{i=1}^{N} e^{-i\beta_m X_i} \prod_{i=1}^{N} e^{-i\gamma_m Z_i Z_{i+1}} | + \rangle^{\otimes N}$$

because $\mathscr{T}_U[Y_i] = \dfrac{1}{|\mathcal{S}|} \sum_{s\in\mathcal{S}} U_s Y_i U_s^{\dagger} = \dfrac{1}{2}\left(Y_i + \mathrm{P} Y_i \mathrm{P}\right) = 0$



Equivariance can help for Barren Plateaus too:



THANKS FOR YOUR ATTENTION!