SKIDMORE COLLEGE
DEPARTMENT OF PHYSICS

PRESENTED AT
Faculty Student Summer Research Program (2026)

PHASES OF QUANTUM D_N THEORIES VIA NEURAL QUANTUM STATES

Adam Blyberg '27, Marta Insolia '27, Anthony Ashmore

MOTIVATION: D_N SPIN CHAINS

Physical systems are often governed by symmetry. The most interesting cases are real physical systems with **non-abelian** symmetry.

We used neural networks to study quantum spin chains with **dihedral (D_N) symmetry** – rotations + reflections of a regular N-gon – one of the simplest non-abelian symmetry groups. We focus on the D_3 group.

Goal: build a neural network that models the ground-state wavefunction, using the non-abelian structure of D_3 rather than treating group elements as arbitrary unrelated integers.

Closest reference: O'Brien & Fendley study a three-state spin model with D_3 symmetry [1]. Our work tackles the **full group** on each lattice site.

THE GROUP AND THE HILBERT SPACE

D_3 has six elements: the **identity** e, two **rotations** $\{r, r^2\}$ and three **reflections** $\{s, rs, r^2s\}$, with group relations

$$r^3 = e, \qquad s^2 = e, \qquad srs = r^{-1}.$$

Basis convention:

$$0 = e, \quad 1 = r, \quad 2 = r^2, \quad 3 = s, \quad 4 = rs, \quad 5 = r^2s$$

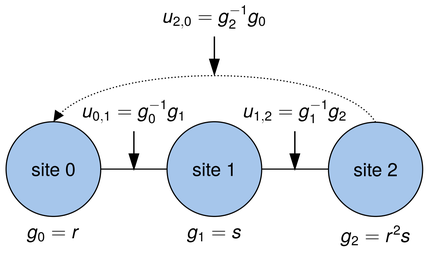
Each of the L chain sites carries a basis state $|g_i\rangle$ for $g_i \in D_3$ – the full Hilbert space is the group algebra tensored over the chain,

$$\mathcal{H} = \mathbb{C}[D_3]^{\otimes L}, \qquad \dim \mathcal{H} = 6^L.$$

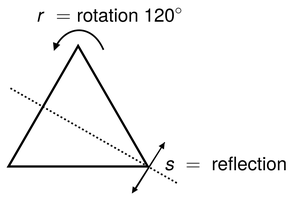
Example state for $L = 3$:

$$|\psi\rangle = |r\rangle \otimes |s\rangle \otimes |r^2s\rangle.$$

We assume periodic boundary conditions throughout.



A D_3 spin chain with $L = 3$ sites, periodic boundary conditions.



The group D_3 acts on a regular 3-gon, i.e. an equilateral triangle.

THE HAMILTONIAN: TWO KINDS OF LOCAL TERMS

Bond terms: Diagonal, two-site operators that detect the conjugacy class of the relative element $u_{i,i+1} = g_i^{-1}g_{i+1}$. Extending to the whole chain gives:

$$H_e = \sum_i \Pi^e_{i,i+1}, \qquad H_r = \sum_i \Pi^r_{i,i+1}, \qquad H_s = \sum_i \Pi^s_{i,i+1}.$$

$$D_3 = \{e,\ r,\ r^2,\ s,\ rs,\ r^2s\}, \qquad C_e = \{e\}, \quad C_r = \{r, r^2\}, \quad C_s = \{s, rs, r^2s\}.$$

Transverse terms: Off-diagonal, single-site operators that act by left multiplication at one site and are summed over full conjugacy classes.

$$H_{L_r} = \sum_i \left(L_r + L_{r^2}\right)_i, \qquad H_{L_s} = \sum_i \left(L_s + L_{rs} + L_{r^2s}\right)_i.$$

Hamiltonian: The energy of the system is determined by

$$H = g_e H_e + g_r H_r + g_s H_s + g_{L_r} H_{L_r} + g_{L_s} H_{L_s},$$

H admits a $D_3 \times D_3$ **global symmetry**: the same $(h_L, h_R) \in D_3 \times D_3$ applied at every site simultaneously, implemented by

$$U_L(h) = \bigotimes_i L_h^{(i)}, \qquad U_R(h) = \bigotimes_i R_h^{(i)}.$$

The Hamiltonian is **invariant** under the symmetry, so the ground state **transforms** under the symmetry.

FINDING THE GROUND STATE

Exact diagonalization: The ground state wave-function captures interesting properties of the system (physics + phase transitions). For short chains, we can find this exactly, but this method becomes intractable for larger chains as the dimension of the Hilbert space grows as 6^L.

$$\text{e.g.} \quad \dim \mathcal{H} = 6^{20} \approx 10^{15}.$$

Just storing the ground state as a vector is out of reach.

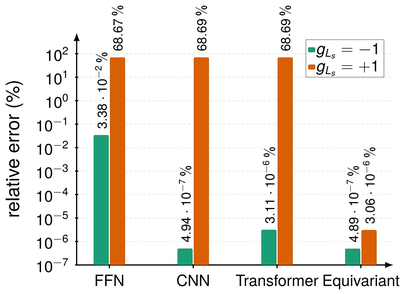
NEURAL QUANTUM STATES (NQS)

Represent the wavefunction directly as a neural network: $\sigma \mapsto \langle \sigma | \psi_\theta \rangle = \psi_\theta(\sigma)$, with the network's weights θ as variational parameters [2].

- Training = minimizing the energy of ψ_θ with gradient descent.
- The lowest-energy state the network can reach is its best approximation of the ground state.
- Implemented using **NetKet** [3], with configurations sampled by **Monte Carlo**.
- We first used networks without built-in symmetry, but realized that the group structure was crucial.

THREE BASELINE NETWORKS (NON SYMMETRY-AWARE)

Tested three architectures: **FFN**, **CNN** and **Transformer**. Each network receives the raw integer labels $0, \ldots, 5$, with no group structure built in.



The takeaway:

- The three baseline networks must infer the D_3 multiplication rules during training – CNN seems to do best at this.
- The three baseline networks fail badly for positive g_{L_s} values.

TOWARD A GROUP-EQUIVARIANT NETWORK

Inspired by Favoni et al. [4], we constructed a group-equivariant network.

To make the network $D_3 \times D_3$-equivariant, we do not treat group elements as raw integer labels. Instead, we encode the relevant group elements using their 2×2 matrix representations. For example,

$$\rho(r) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \qquad \rho(rs) = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}, \qquad \theta = \frac{2\pi}{3}.$$

The hidden layers multiply these matrices together, so the computations are equivariant by construction. The output layers use traces and determinants to extract scalars.

Result: The group structure is built into the network rather than something the network has to learn from data. The network can represent wavefunctions transforming trivially under the $D_3 \times D_3$ symmetry.

THE SIGN PROBLEM

Our network outputs a single complex number – the probability amplitude $\psi_\theta(\sigma)$ – so the wave-function's magnitude and its sign have to be learned together. This can be hard for $g_{L_s} > 0$ as the sign of $\psi_\theta(\sigma)$ flips in a very sharp, non-local way. This is known as a **sign problem**.

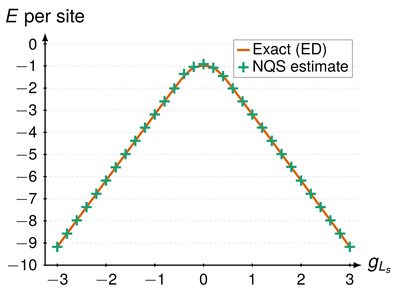
Following Szabó et al. [5], we found the D_3-specific source of our sign problem and solved it with a simpler mechanism than their two-network split:

The fix: `sign_gate`

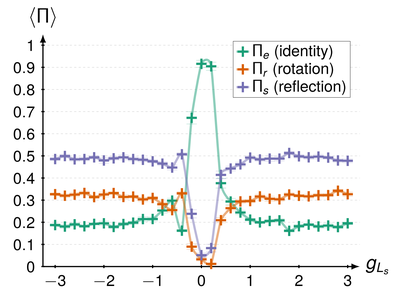
- D_3's natural $\pm$ sign: $\chi_i = +1$ on rotations, $\chi_i = -1$ on reflections.
- Chain-wide: $\chi(\sigma) = \prod_i \chi_i(g_i) = (-1)^{\#\text{reflections}}$.
- Learn one complex weight w that gates whether to use $(-1)^{\#\text{reflections}}$ or not.

Result: The network learns when to use the non-local information to correctly model the non-trivial sign structure.

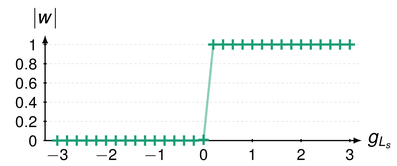
RESULTS



Ground-state energy per site vs g_{L_s}: NQS estimate compared to exact diagonalization.



Bond-class fractions (Π_e, Π_r, Π_s) vs g_{L_s}.



`sign_gate` weight vs g_{L_s}.

Sign Gate: $|w|$ is the weight on the explicit sign-character correction. It sits at zero for $g_{L_s} < 0$ and jumps to one for $g_{L_s} > 0$. The gate learns and accounts for the sign structure.

FUTURE DIRECTIONS

- Improve the network further – target non-trivial **sign** or **standard** representations directly, rather than only the trivial one.
- Compute observables that distinguish the different phases and map out the full **phase diagram**.
- Extend the construction to D_N for general N and explore how the phase structure changes.

References

[1] E. O'Brien and P. Fendley, "Self-dual S_3-invariant quantum chains", *SciPost Phys.* **9** (2020)088, arXiv:1912.09464 [cond-mat.stat-mech].

[2] G. Carleo and M. Troyer, "Solving the quantum many-body problem with artificial neural networks", *Science* **355** 6325, (2017)602–606, arXiv:1606.02318 [cond-mat.dis-nn].

[3] F. Vicentini *et al.*, "NetKet 3: Machine Learning Toolbox for Many-Body Quantum Systems", *SciPost Phys. Codeb.* **2022** (2022)7, arXiv:2112.10526 [quant-ph].

[4] M. Favoni, A. Ipp, D. I. Müller, and D. Schuh, "Lattice Gauge Equivariant Convolutional Neural Networks", *Phys. Rev. Lett.* **128** 3, (2022)032003, arXiv:2012.12901 [hep-lat].

[5] A. Szabó and C. Castelnovo, "Neural network wave functions and the sign problem", *Phys. Rev. Res.* **2** (2020)033075, arXiv:2002.04613 [cond-mat.str-el].