ICCUB
Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA

EXCELENCIA MARÍA DE MAEZTU 2020-2023

UNIVERSITAT DE BARCELONA

Symmetries in Neural Quantum States

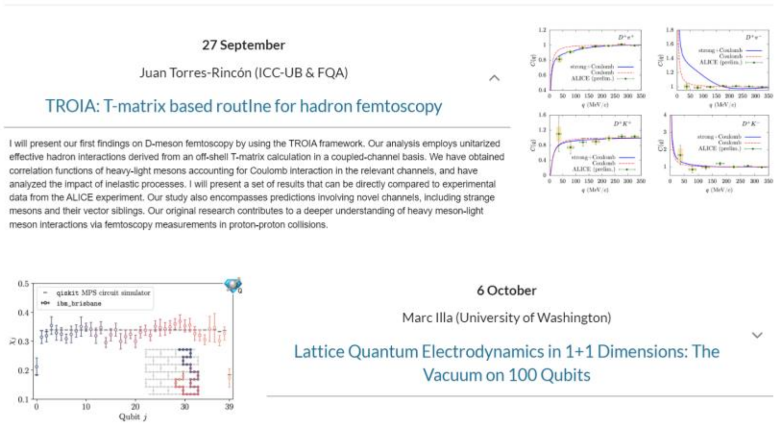
Javier Rozalén Sarmiento

Advisor: Arnau Rios Huguet

The Hadronic, Nuclear and Atomic Physics Group (∈ FQA)

People

HadNuc@UB Seminars



27 September

Juan Torres-Rincón (ICC-UB & FQA)

TROIA: T-matrix based routIne for hadron femtoscopy

I will present our first findings on D-meson femtoscopy by using the TROIA framework. Our analysis employs unitarized effective hadron interactions derived from an off-shell T-matrix calculation in a coupled-channel basis. We have obtained correlation functions of heavy-light mesons accounting for Coulomb interaction in the relevant channels, and have analyzed the impact of inelastic processes. I will present a set of results that can be directly compared to experimental data from the ALICE experiment. Our study also encompasses predictions involving novel channels, including strange mesons and their vector siblings. Our original research contributes to a deeper understanding of heavy meson-light meson interactions via femtoscopy measurements in proton-proton collisions.

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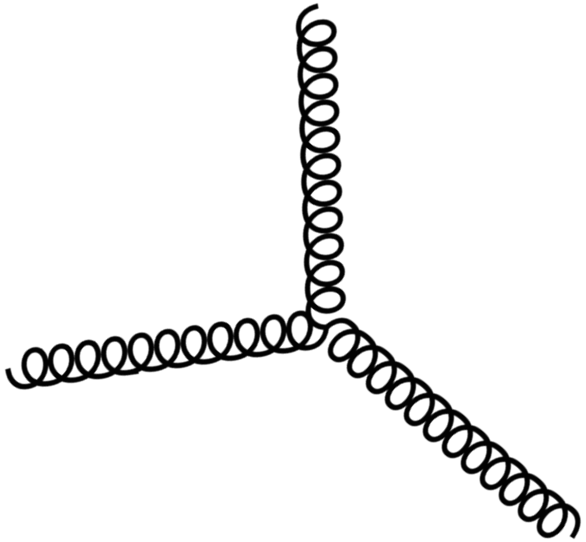
Marc Illa (University of Washington)

Lattice Quantum Electrodynamics in 1+1 Dimensions: The Vacuum on 100 Qubits



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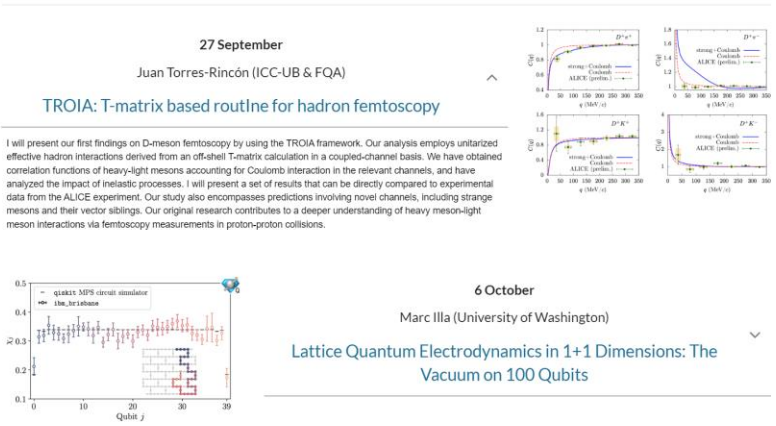

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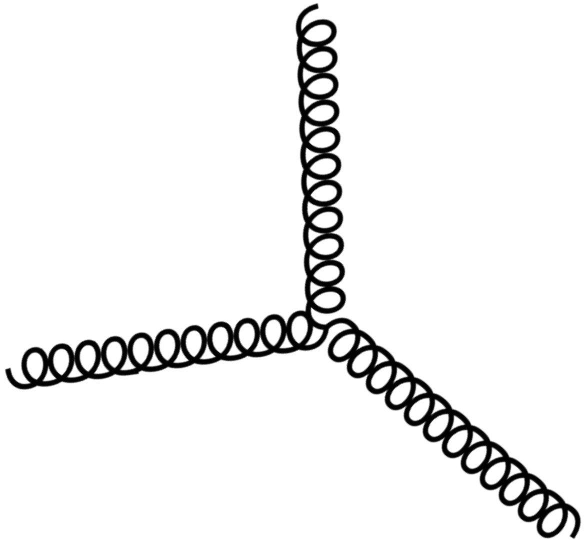

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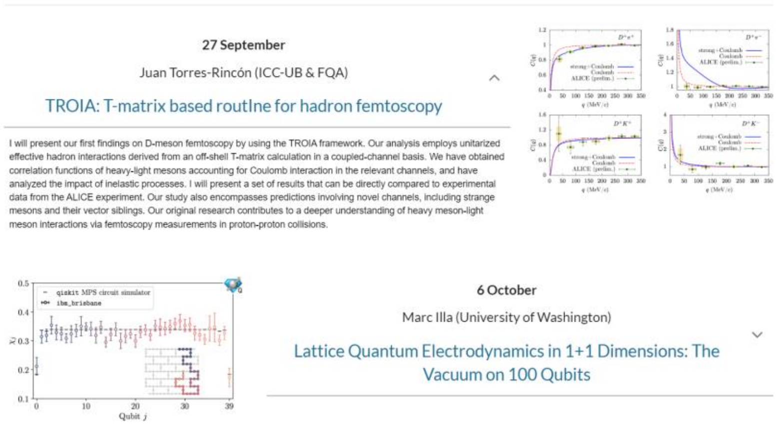

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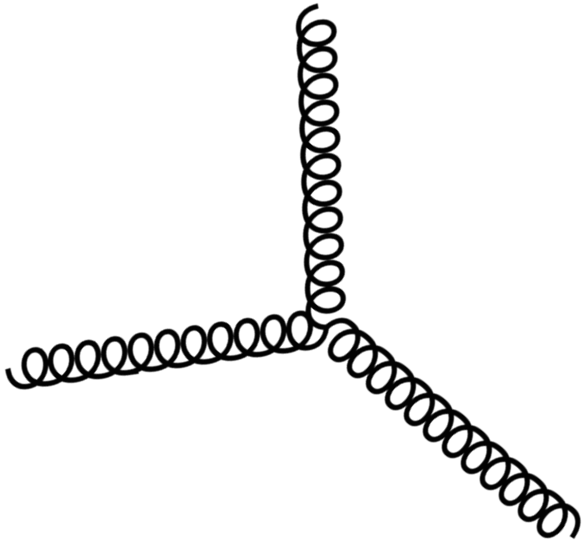

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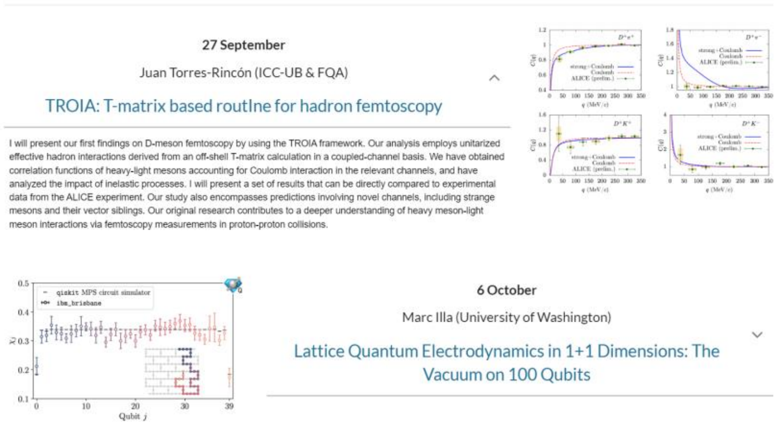

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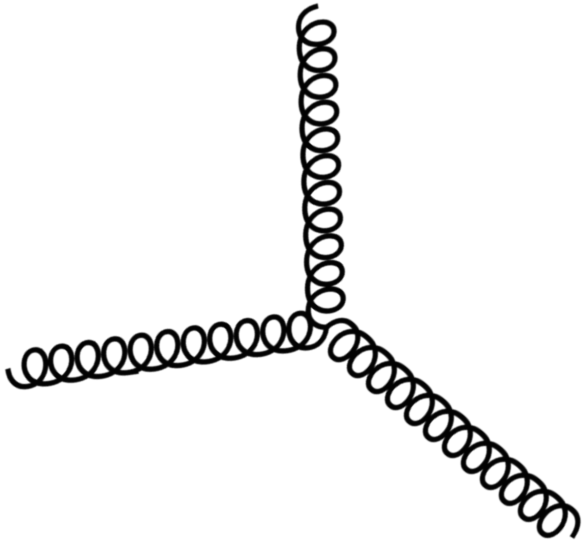

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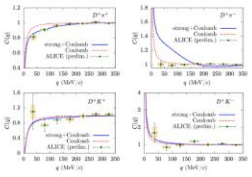

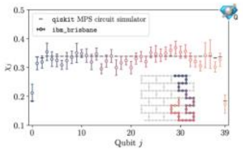

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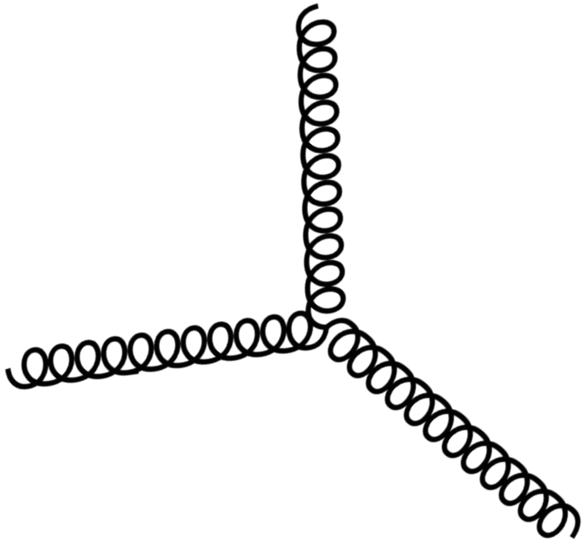

ICCUB has ≈ 80 PhDs & Postdocs (as of 2022)

PhD/PostDoc Students

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Dark Matter detection: baryonic DM interacts with nuclei!

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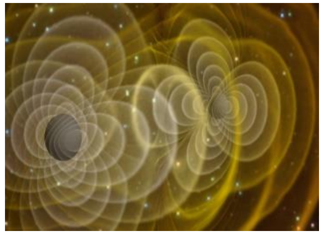

Gravitational waves: strong interaction determines the GW signal in NS mergers

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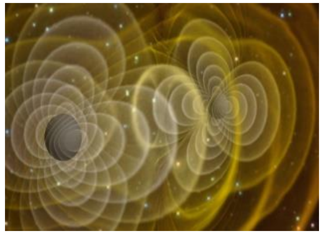
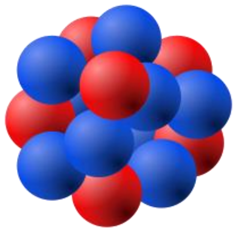


Gravitational waves: strong interaction determines the GW signal in NS mergers

Nuclear structure: static properties of nuclei

The Quantum Many-Body Problem

- **Goal**: Solve for the wave function of an atomic nucleus, ψ



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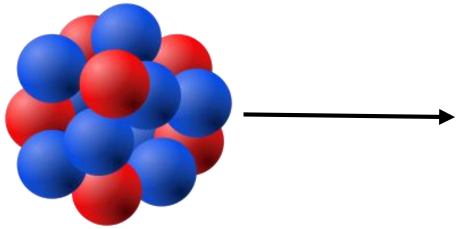

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- **How?** Rayleigh-Ritz variational principle

$$\frac{\langle\psi_\theta|\hat{H}|\psi_\theta\rangle}{\langle\psi_\theta|\psi_\theta\rangle} \geq E_{\mathrm{GS}}$$

$$|\psi_\theta\rangle = \int |p\rangle\, \psi_\theta(\boldsymbol{p_1}, \boldsymbol{p_2}, \ldots, \boldsymbol{p_N})\mathrm{d}^{3\mathrm{N}}\mathrm{p}$$

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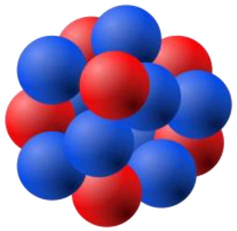

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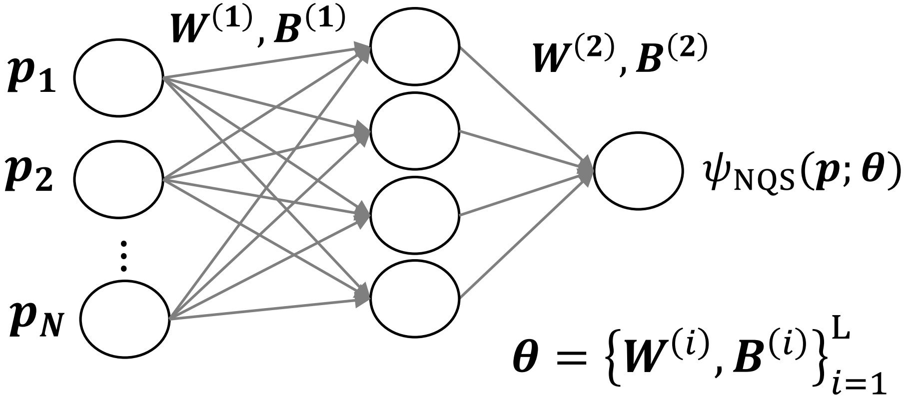
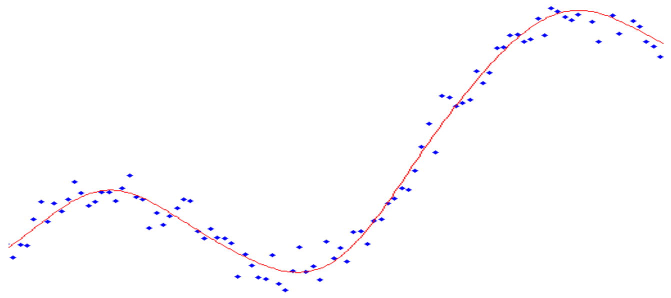
- **NQS Ansatz:** $\psi_{\mathrm{NQS}}(\boldsymbol{p_1}, \boldsymbol{p_2}, \dots, \boldsymbol{p_N}, ; \boldsymbol{\theta})$



Why Neural Networks?

- **NNs have "∞ power"**: a neural network can approximate any continuous function [1], [2].



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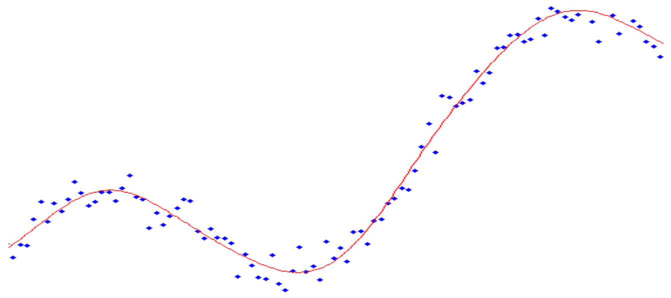
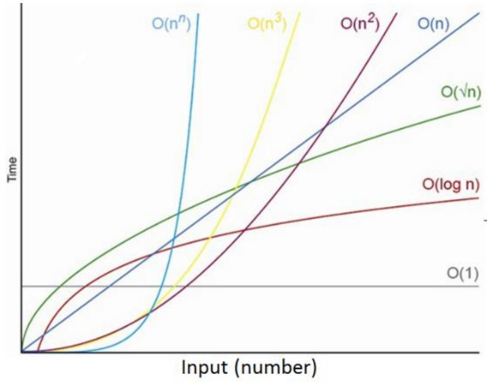


- **Space complexity:** polynomial scaling of memory resources… possibly!



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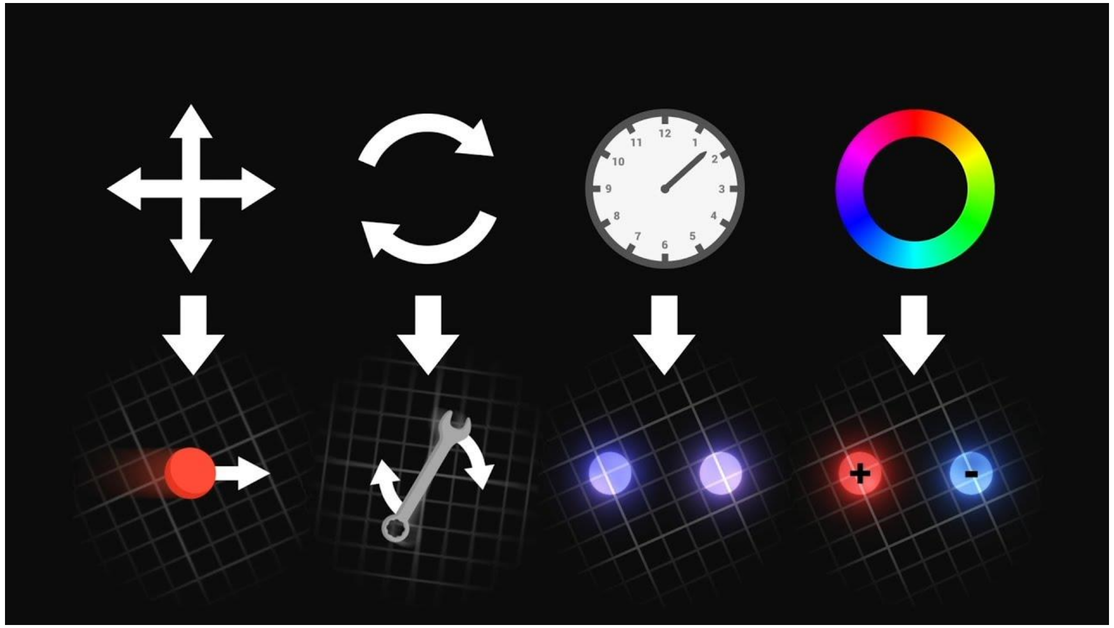
Physics-Inspired Neural Networks

Encoding physics in NNs: symmetries of $\hat{H}$, boundary conditions, etc.

My current work!



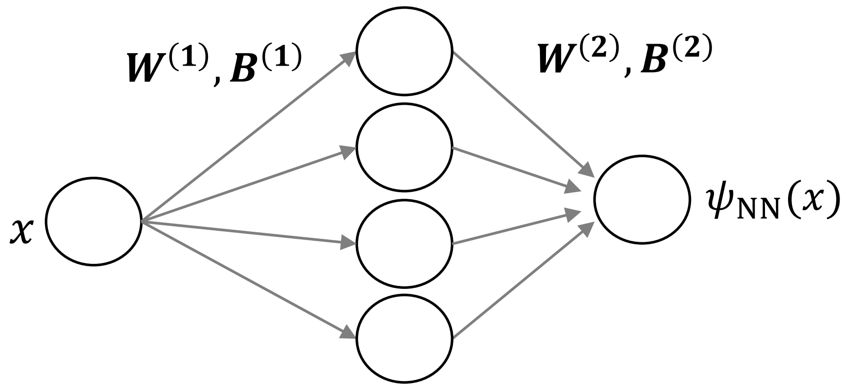
https://www.youtube.com/watch?v=hF_uHfSoOGA&ab_channel=ScienceClicEnglish

Symmetries in neural networks

1D HO: naive approach (but good!)

$$\hat{H} = -\frac{1}{2}\nabla^2 + \frac{1}{2}mw^2\hat{x}^2 \longrightarrow \psi(x) = \pm\psi(-x)$$

$$\psi_{\mathrm{NQS}}(x) \coloneqq \psi_{\mathrm{NN}}(x) \pm \psi_{\mathrm{NN}}(-x)$$



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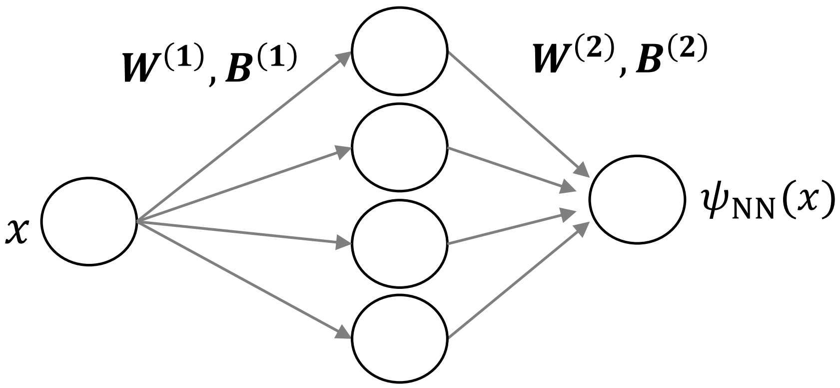
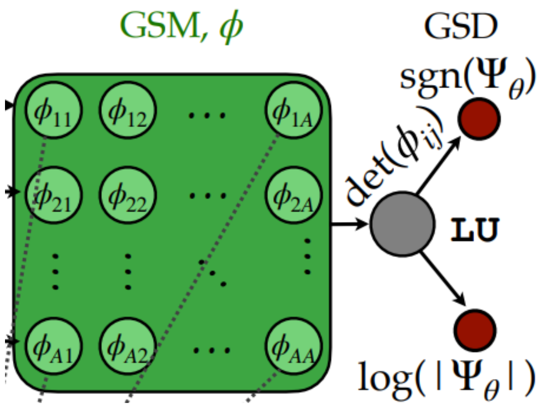


Fermionic particle exchange: common approach

Spin-statistics theorem $\longrightarrow$

$$\psi(\boldsymbol{x_1}, \dots, \boldsymbol{x_i}, \dots, \boldsymbol{x_j}, \dots, \boldsymbol{x_N}) = \pm\psi(\boldsymbol{x_1}, \dots, \boldsymbol{x_j}, \dots, \boldsymbol{x_i}, \dots, \boldsymbol{x_N})$$

$$\psi_{\mathrm{NQS}}(x_1, x_2, \dots, x_N) = \varphi_{\mathrm{EQUIV}} \circ \det \phi_{\mathrm{GSM}}(x_1, x_2, \dots, x_N)$$



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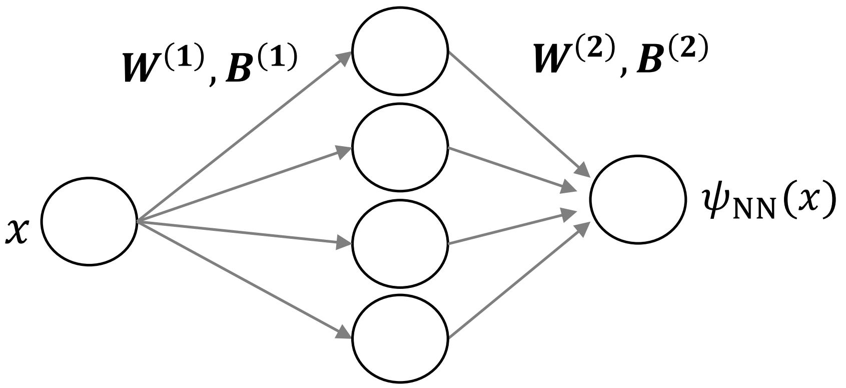

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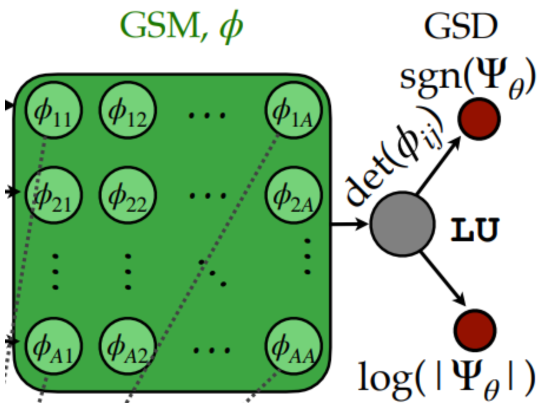

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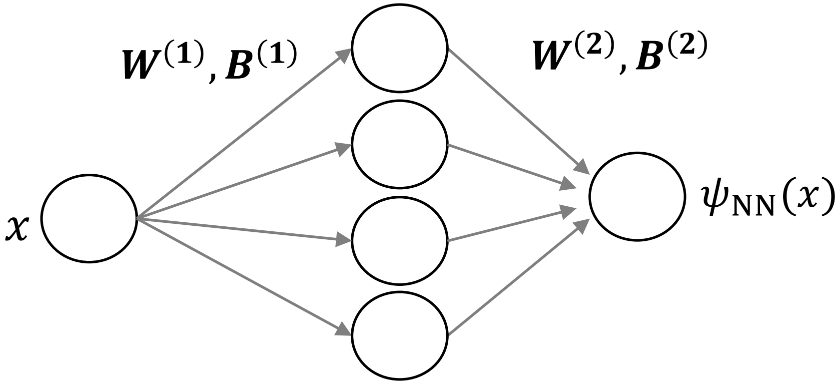

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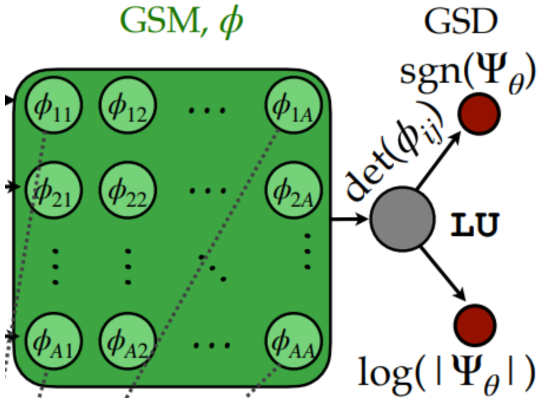

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What about other symmetries (continuous groups)?

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Convolution is all you need

Φ is **equivariant** under a group G if:

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Group convolution $\Leftrightarrow$ Group equivariance (2016-2018) [4, 5, 6]

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Should we design NQSs within this framework?

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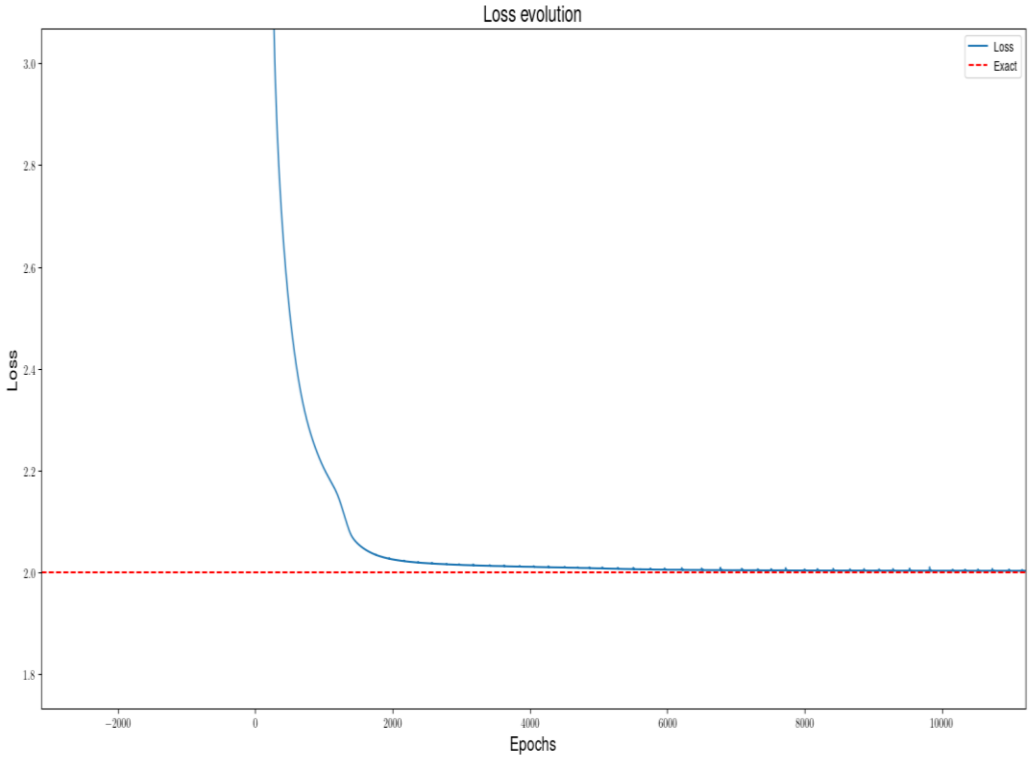
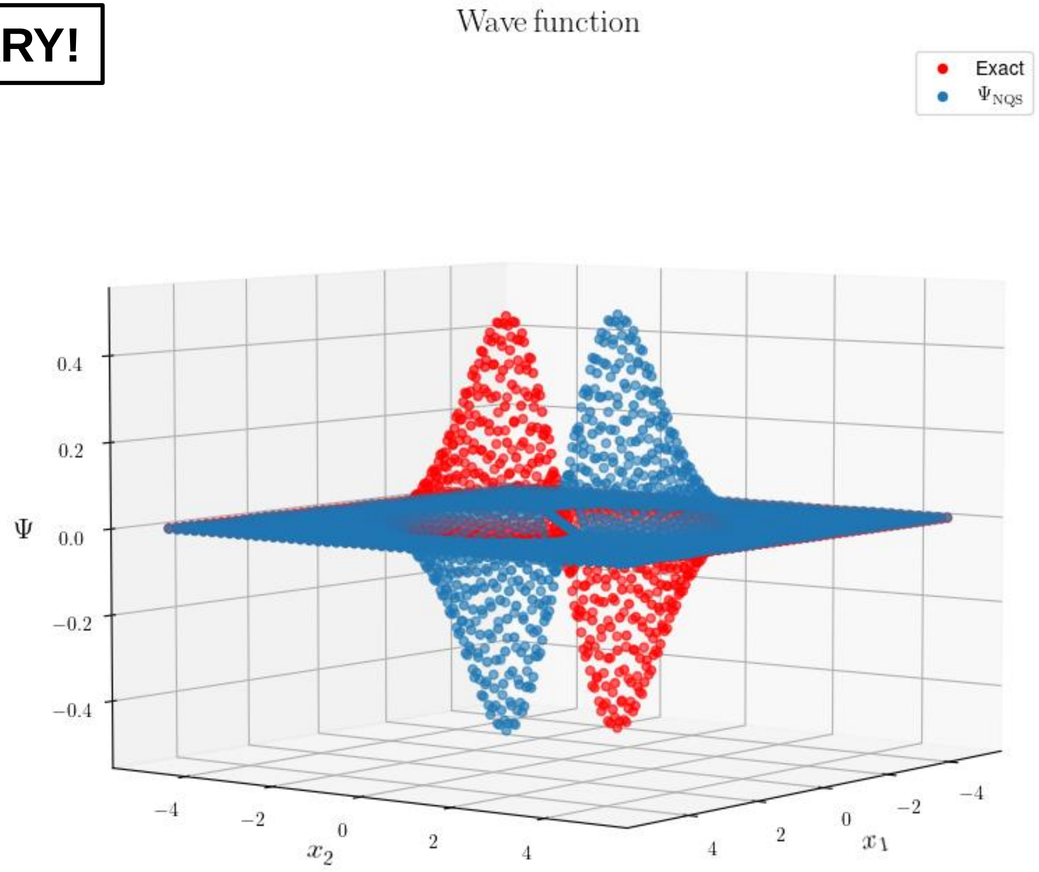
Toy exemple: $G = S_N$

$N = 2$, 1D HO

1 conv layer w/ bias → # weights = $k(|G| + 1 + |G|dN)$ $k = 25, |G| = 2, d = 1$

PRELIMINARY!





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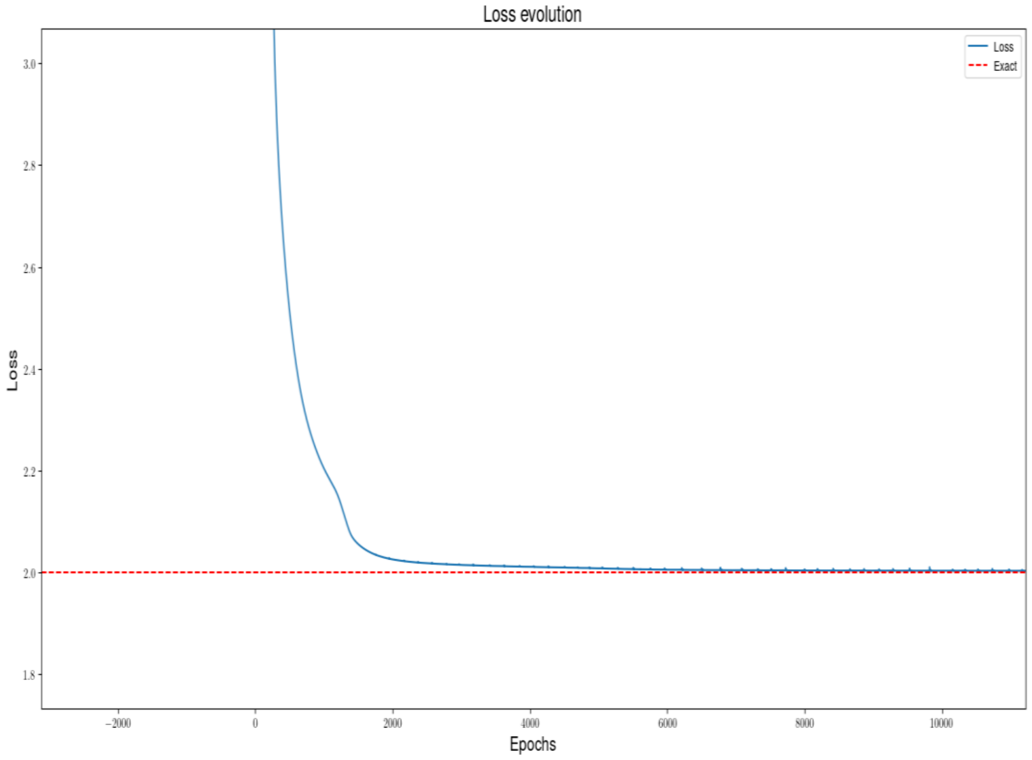

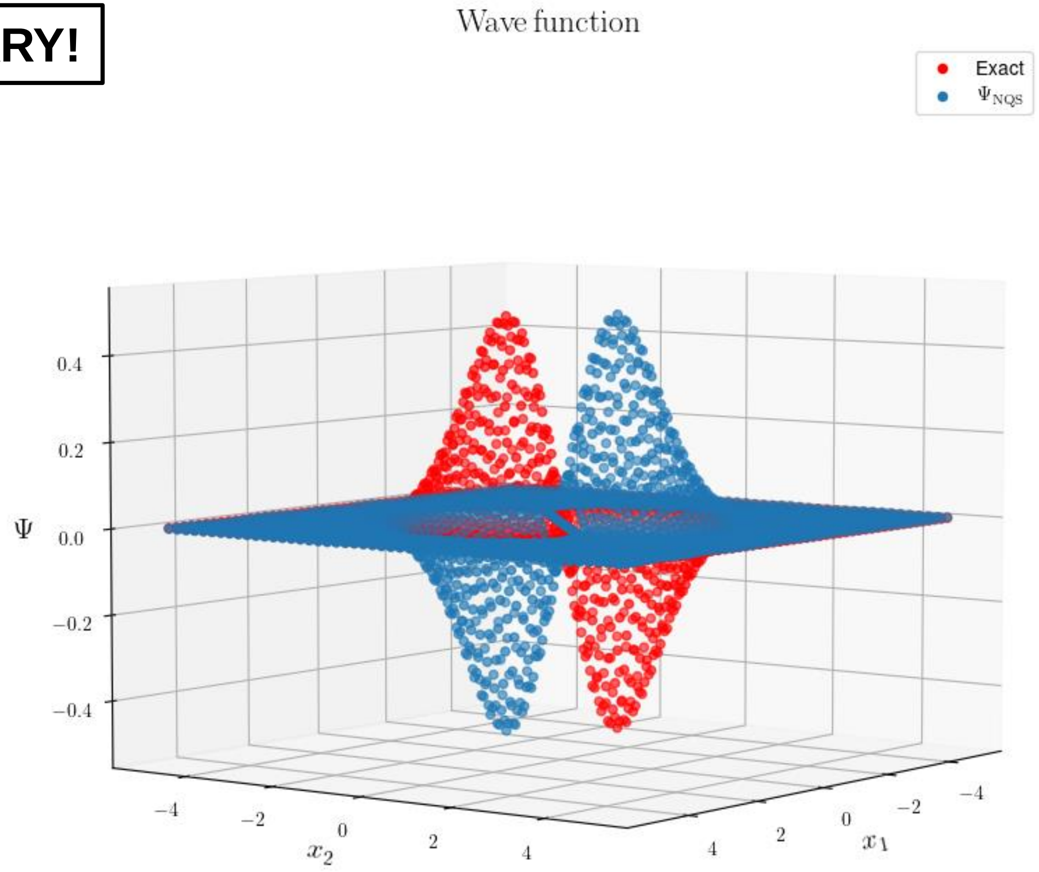

Memory grows factorially with N ☹

Next steps and open questions…

- Why is the Slater “so good”? Can we explain it from the irreps of S_N? Can we find something even better?

- Can we compute any excited state?

- What about continuous groups ($\mathrm{SU(N)}$)?

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