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Symmetries in Neural Quantum States

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Neural Quantum States are at the basis of a new ab-initio method especially designed to tackle the quantum many-body problem. These combine the variational method with neural networks, a flagship tool of modern Machine Learning. Neural Quantum States have been successfully used in spin, electronic and nuclear many-body systems. Neural networks can provide an unbiased approximation of complex wave functions, and so far the growth of network parameters with particle number has been found to be polynomial. One expects the growth to be further mitigated by restricting ansätze to the manifold of states that respect physical symmetries. To this end, starting from the most general way to make a neural network equivariant to a certain symmetry group, we design a many-body neural network ansatz which respects the fermionic particle-exchange symmetry. Previous fermionic ansätze are a specific case of this general approach, which we develop formally, foreseeing the need to develop relevant nuclear symmetries, like spin and isospin, into a Neural Quantum State. I will discuss how this approach will be exploited in future nuclear physics simulations and show some initial results on test systems.

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