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Fachbereich Physik, Universität Stuttgart
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Machine Learning for the Many-Electron Problem

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Abstract

Since their introduction [1], neural-network parameterizations of the many-body wave function have been succesfully used to study model hamiltonians, e.g. on prototypical frustrated spin models. In this presentation I will discuss recent strides in using neural quantum states for the ab-initio study of the many-electron problem, from molecules [2] to periodic systems. I will delve into a message-passing-neural-network-based Ansatz designed for simulating strongly interacting electrons in continuous space [3]. This approach achieves high accuracy in the homogeneous electron gas problem, pushing the boundaries of system sizes previously inaccessible to other neural-network based architectures such as FermiNet. I will also discuss a Pfaffian-based neural-network quantum state for ultra-cold Fermi gases, outperforming traditional methods and enabling exploration of the BCS-BEC crossover region [4]. Finally, I will discuss ongoing work in extending neural network representations to study many-electron dynamics [5] and finite temperature properties.

[1] Carleo and Troyer, Science 355, 602 (2017)
[2] Hermann et al., Nature Reviews Chemistry 7, 692 (2023)
[3] Pescia et al., Phys. Rev. B 110, 035108 (2024)
[4] Kim et al., arxiv:2305.08831 (2023)
[5] Nys, Pescia, Sinibaldi, and Carleo, Nat. Comm. 15, 9404 (2024)