# Machine Learning and Neural Networks for Quantum Systems

**Antoine Georges**

*Collège de France, Paris and Flatiron Institute, New York*
antoine.georges@college-de-france.fr

Learning algorithms using deep neural networks are currently having a major impact on basic sciences. The physics of complex quantum systems is no exception, with multiple applications that constitute a new field of research. Examples include the representation and optimization of wave functions of quantum systems with large numbers of degrees of freedom (neural quantum states), the determination of wave functions from measurements (quantum tomography), and applications to the electronic structure of materials, such as the determination of more precise density functionals or the learning of force fields to accelerate molecular dynamics simulations. I will survey some of these applications, with an emphasis on neural quantum states.

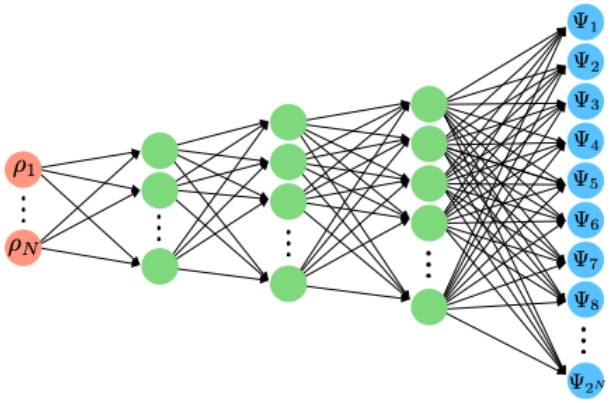


**Figure 1:** Machine learning the Hohenberg-Kohn correspondence: a neural network learning the wave-function of a many-body quantum systems from the knowledge of the local charge density [Adapted from J.Robledo-Moreno, G.Carleo and A.Georges Physical Review Letters 125, 076402 (2020).

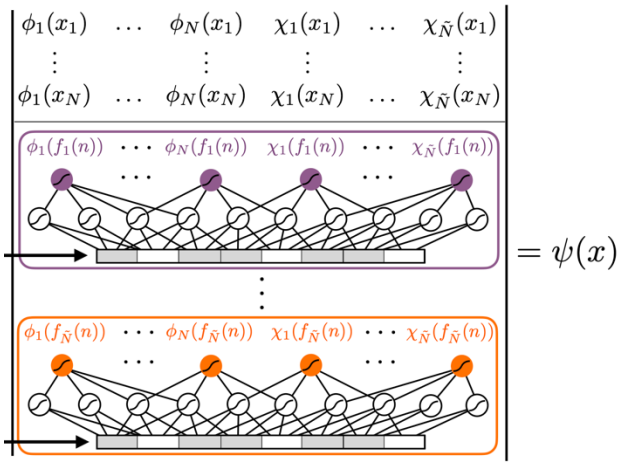


**Figure 2:** A `Neural Quantum State' using hidden fermions [Adapted from J.Robledo-Moreno, G.Carleo, A.Georges and J.Stokes, PNAS 119, e2122059119 (2022)

## References

Antoine Georges, Cours au Collège de France, 2022-23

## Figures