Contribution ID: **40**   Type: **not specified**

Machine learning for reduced density matrix functional theory

Wednesday, 12 October 2022 10:30 (30 minutes)

The one-body reduced density matrix (1RDM) plays a fundamental role in describing and predicting quantum features of bosonic and fermionic systems, such as Bose-Einstein condensation. Based on a decomposition of the 1RDM, we have developed a method to design reliable approximations for such universal functionals: Our results suggest that for translational invariant systems the constrained search approach of functional theories can be transformed into an unconstrained problem through a parametrization of a Euclidian space. This simplification of the search approach allows us to use standard machine learning methods to perform a quite efficient computation of both the universal functional and its functional derivative. For the Bose-Hubbard model, we present a comparison between our approach and the quantum Monte Carlo method.

This talk is based on:
J. Schmidt, M. Fadel, and C. L. Benavides-Riveros, Phys. Rev. Research 3, L032063 (2021).

Presenter: BENAVIDES-RIVEROS, Carlos