Contribution ID: **118** Type: **Talk**

【443】Convolutional Neural Networks as Kinetic Energy in Orbital-free Functional Theory

Thursday, 2 September 2021 15:00 (15 minutes)

The main goal of the project is to find a machine learning approximation for the kinetic energy functional of orbital-free density functional theory,
\begin{equation}
T[n] = \int \tau[n] \,\mathrm{d}x,
\end{equation}

where the function $\tau[n]$ is represented using a feed forward neural network. Since it is known that the function τ is translationally invariant and non-local, i.e. a function of the values of n at various positions x, the structure of a convolutional neural network seems like a reasonable choice.

Primary authors: Prof. HAUSER, Andreas (Graz University of Technology - Institute of Experimental Physics); LUKIC, Daniel (Graz University of Technology); Dr RALF, Meyer

Presenter: LUKIC, Daniel (Graz University of Technology)

Session Classification: Atomic Physics and Quantum Optics

Track Classification: Atomic Physics and Quantum Optics