Contribution ID: **23** Type: **Short Talk**

Modelling quantum states using normalizing flows

Friday, 25 November 2022 11:30 (10 minutes)

The solution of the time-dependent Schrödinger equation completely characterizes the quantum dynamics of molecular systems. Because this equation is analytically solvable only for toy problems, for real-life simulations, a variety of numerical approximations have been developed. The most accurate methodologies employ the variational approach based on the linear expansion of the solutions in a set of basis functions. Recently, neural network approaches have emerged as a strong methodology for modeling the basis functions, which prove very efficient for solving quantum chemical problems.

I will present a novel approach for solving the stationary and time-dependent Schrödinger equation based on normalizing flows and invertible neural networks acting on the problem's real-space coordinates. In this method, instead of using neural networks as a basis, a set of classical orthogonal polynomials is composed together with a neural network function. This allows us to calculate a much larger number of excited states at a much lower cost. I'll present calculations for excited electronic and vibrational states of small molecules. To solve the time-dependent problems, the current approach is to cast in the form of a recurrent neural network that describes the molecular state on a discretized time lattice. This method will be used as a workbench for simulations of the Laser Induced Electron Diffraction (LIED) experiments, a technique for high spatial and temporal resolution imaging.

Primary authors: FERNANDEZ CORRAL, Alvaro (FS-CFEL-CMI (CFEL-CMI Controlled Molecule Imaging)); YACHMENEV, Andrey (FS-CFEL-1-CMI (CFEL-CMI Controlled Molecular Imaging)); SALEH, Yahya (FS-CFEL-1-CMI (CFEL-CMI Controlled Molecular Imaging))

Presenter: FERNANDEZ CORRAL, Alvaro (FS-CFEL-CMI (CFEL-CMI Controlled Molecule Imaging))