Machine Learning for quantum dynamics

Kanishka Singh

3rd year PhD student in Machine Learning & Theoretical Chemistry

HEIBRIDS data science school & Helmholtz Zentrum Berlin

Wave packet propagation is crucial to understanding time-dependent quantum phenomena such as nuclear dynamics, chemical reactions, and spectroscopy. Multi Configuration Time Dependent Hartree (MCTDH) approach has been extensively used to understand and simulate such processes. However, the MCTDH approach has a few limitations, such as the speed of calculations, and the accumulation of errors over large timescales of simulation. In our work, we demonstrate that Fourier Neural Operators, an emerging approach used in Machine Learning to solve differential equations, can be trained to propagate wave packets in different 2-dimensional potentials. Once trained over a set of potentials of the same functional form, our method can predict accurately, the propagation over a similar novel potential, thereby demonstrating the capture of an understanding of the underlying dynamics of propagation. We further demonstrate that such low-cost surrogate machine learning models provide a useful option to generate low-cost simulations of chemical phenomena and estimate wave packet and potential parameters, which can then be used for exact high-accuracy calculations using quantum chemical methods such as MCTDH