

Title: Enhancing scattering theory with machine learning

Abstract: I will describe our recent work exploring how AMO physics theory, and in particular calculations of quantum dynamics of atoms and molecules, can benefit from machine learning. The particular focus will be on Bayesian methods with applications aiming to infer as much information from as little physical data as possible. Traditionally, quantum theory views atoms as undergoing dynamics on a given potential energy surface. I will describe and advocate an approach that formulates quantum dynamics problems as the Schrödinger equation with a non-parametric distribution of potential energy surfaces that becomes conditioned by the desired dynamical properties (such as the experimental measurements). For more details, see: PCCP 21, 13392 (2019); NJP 21, 022001 (2019); PRL 121, 255702 (2018).