Extending Greens Function using Machine Learning in Time and Space

Hubert Pugzlys[1], Huy Tran[1], Sam Dillion[1], Shuyi Li[1], Xuzhe Ying[2], and Chunjing Jia[1]

[1]*Department of Physics, University of Florida, Gainesville, FL 32611, United States*
[2]*Department of Physics, Hong Kong University of Science and Technology, Hong Kong*

Obtaining the spectrum and dynamical responses of quantum materials can be fundamental to microscopic understanding of their physical properties. For quantum magnetism, the dynamical responses of certain simple systems can be calculated analytically; however, this cannot be acquired for numerous complex many-body systems. While numerical methods, such as exact diagonalization and density matrix renormalization group, exist for such systems, the time evolution algorithms often propagate errors that depreciate the accuracy of the spectra at long time and space intervals. In addition, the computational cost of these numerical methods drastically increases with the size of the system, preventing us from studying systems approaching the thermodynamic limit. In this project, we employ machine learning algorithms to extend the dynamical spin correlations in both temporal and spatial dimensions with improved resolution. We train the models using Time-dependent Density Matrix Renormalization Group (tDMRG) simulated for XXZ model on a finite-size one-dimensional lattice. We benchmark our machine learning obtained spin dynamical correlation results against those obtained from analytical calculations of solvable models such as the XXZ model. After assessing the accuracy of our machine learning model, we hope to analyze other strongly interacting many-body systems that do not have an analytical solution using this method. This method aims to enhance the understanding of the dynamical spin correlation with much higher resolution, and for systems approaching the thermodynamic limit.