Transformer-based Neural Quantum States for Quantum Impurity Models

Quantum impurity models (QIMs) are crucial for understanding strongly correlated systems and are foundational to dynamical mean-field theory. Despite substantial progress, solving QIMs with many internal degrees of freedom remains computationally challenging, especially for multi-orbital systems relevant to transition-metal and rare-earth compounds. In this study, we employ transformer-based neural quantum states to parameterize the many-body wave function of QIMs, leveraging their capacity to capture long-range correlations and entanglement. By representing QIMs in the natural orbital basis, we develop an expansion scheme for optimizing these states with efficiency and accuracy surpassing traditional variational Monte Carlo methods, enabling precise treatment of complex QIMs. Additionally, we propose an innovative technique for the efficient calculation of core-level X-ray absorption and photoemission spectra (XAS/XPS) in QIMs, providing direct access to experimentally relevant observables.