ABSTRACT

Understanding the collective behavior of many-body quantum systems is crucial for exploring phenomena such as metal-insulator transitions, bound complexes, superconductivity, and magnetism. The standard approach for studying these systems is through Green's functions, mainly few-body Green's function, which provides insights into excitations in a many-body ground state. The Lanczos method and Density Matrix Renormalization Group (DMRG) are commonly used for studying ground-state properties. However, challenges arise in addressing phenomena like many-body localization, bound complexes, and chaos in few-body systems, where the total many-body density of states (DOS) is crucial. Existing methods like Lanczos and DMRG are limited to ground-state and a few excited states. Hence, Exact diagonalization (ED) is the only viable method for such problems, but the exponential growth of the Hilbert space poses computational challenges in terms of memory and time requirements.

The present thesis explores a fundamental issue in many-body systems: accurately computing the exact many-body Green's function and few-body excitations with reduced computational resources. To address this challenge, we have developed a new many-body technique, the 'Fock space recursive Green's function' method (F-RGF). For a many-body problem with $\mathcal{L}$ site and $\mathcal{N}$ spinless fermion, where the Hilbert space grows as ${}^{\mathcal{L}}C_{\mathcal{N}}$, we have demonstrated that F-RGF leads to $O(1/\mathcal{L})$suppression in memory and time complexity for computing many-body Green's function compared to brute force methods. We have benchmarked F-RGF against exact diagonalization and shown that F-RGF conserves the many-body spectral sum rule. We have derived relations to extract few-body correlation functions from the many-body Green's function and have applied the method to few-body spectroscopies. These include two-hole spectral functions relevant to Auger electron spectroscopy (AES), which reveals information about the local electronic structure and allows the extraction of local interaction parameters and multi-spin correlation function related to neutron and resonant inelastic x-ray scattering (RIXS). In the AES study, we have put bounds where the well-known Cini-Sawatzky theory is applicable. We discovered the presence of high-energy spin excitation in the spin half trimer chain by computing up spin correlation functions relevant to RIXS. .