Ab Initio No-Core Shell Model

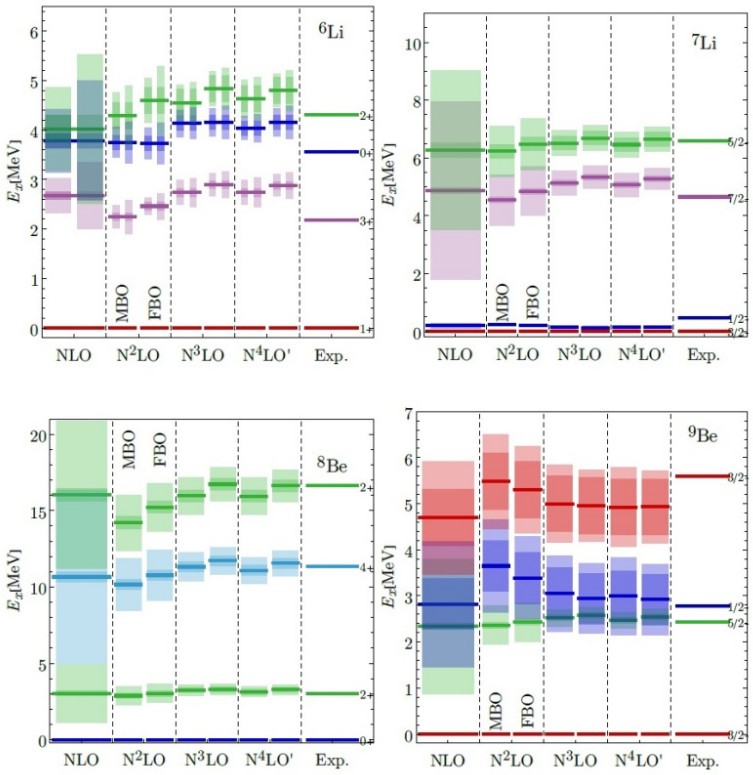


Figure 1: Spectra of selected Li and Be isotopes calculated in IT-NCSM calculations with the MBO and FBO interaction families with $\Lambda = 500$ MeV. The uncertainty bars include many-body (dark) and chiral (light) uncertainty estimates. For ^{6}Li we show the chiral uncertainties estimated with the EKM (left) and Bayesian (right) uncertainty quantification. For the other nuclei, we show only the uncertainties derived with the Bayesian uncertainty quantification.

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Project Term
2021 - 2022

Clusters
Lichtenberg Cluster Darmstadt

Additional Software
Importance-Truncated No-Core Shell Model, ARPACK

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Introduction

The prime goal of ab initio nuclear structure theory is the description of correlated systems of many nucleons based on the fundamental theory of the strong interaction, Quantum Chromodynamics (QCD). On this path, we are faced with two challenges: First, unlike e.g. in atomic physics, the interaction itself is not well-known because it cannot be derived directly from QCD. Second, the quantum many-body problem of the nucleus is especially hard to solve due to the properties of the nuclear interaction and range of particle numbers (from 2 to ~300) that is of interest. While this project focuses on the latter challenge, its results provide valuable feedback on the quality of interactions, supporting efforts tackling the first challenge. The quantum many-body problem is cast into the form of a large-scale eigenvalue problem, with linear matrix dimensions easily reaching 10^9 or 10^{10}. The computation and storage of the many-body matrix elements and the extraction of low-lying eigenvalues and eigenvectors is a clear HPC challenge.

Methods

Methods The methodological back-bone of the research project is the Importance-Truncated No-Core Shell Model (IT-NCSM), one of the modern ab initio many-body methods that was developed in our group. It provides quasi-exact solutions of the many-body Schrödinger equation for nuclei up to mass A ≈ 25 and gives access to the full suite of nuclear structure observables, such as ground-state and excitation energies, radii, electromagnetic transitions and moments, or densities and form-factors. We compute a matrix representation of the Hamiltonian on the importance-truncated basis and extract a small number of the lowest eigenvalues and their eigenvectors using the ARPACK implementation of the Lanczos algorithm. The importance threshold is then raised successively, removing rows and columns from the matrix, and diagonalized again in order to get a sequence of eigenvalues that can be extrapolated to the vanishing threshold. For the IT-NCSM, apart from the importance-truncation scheme itself, this project relies on our developments in computing and handling m-scheme 3N matrix elements. The matrix elements are now stored in a coupled basis and the decoupling to the conventional m-scheme is performed on-the-fly during the NCSM calculation in a very fast and cache-e cient way. Our IT-NCSM code uses a hybrid MPI/OpenMP parallelization scheme to make maximum use of the available memory.

Results

In this project we have performed various NCSM and IT-NCSM calculations of different observables in p-shell nuclei. In particular, we studied the effects of a new family of chiral interactions (see also project 1329) on spectra of light p-shell nuclei as well as the hypernucleus $^{7}_{\Lambda}$Li and took a closer look at the electromagnetic properties of ^{16}C. Furthermore, we have developed new methods for bound states as well as resonance states. In the bound regime this includes the implementation of two-body density matrices which can be adapted to different

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operator structures. For the calculation of nuclear resonances we developed two separate methods. On the one hand, the analyzing continuation of the coupling constant which relies on a complex continuation from bound states to resonances. This method was used to perform several calculations on the resonance states of the tetraneutron. On the other hand, we developed a new single-particle basis which contains single-particle resonances and complex scattering states often called Berggren or Gamow basis. All newly developed methods have been benchmarked successfully and are ready for application and further development in the next project period.

Discussion

The results obtained for p-shell nuclei with the new family of interactions are in very good agreement with experimental data especially when considering theory uncertainty estimations based on Bayesian statistics. The same holds for hypernucleus $^{7}_{\Lambda}$Li providing a solid basis for the hypernuclear work package in the upcoming project period. With the development of two-body density matrices we are now able to simplify calculations of operator matrix elements for the NCSM and got some deeper insights in the importance of translational invariance of these operators. The method of the analytic continuation of the coupling constant provided robust results on the tetraneutron resonance and further developments are shifted to other projects. Moreover, the newly developed Gamov NCSM holds promising first results and will be key in the next periods work on resonances and with that the ongoing extension of the NCSM to continuum degrees of freedom.

Reference

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Last Update: 2022-04-23 15:24