Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Large-Scale Configuration Interaction for Ab Initio Nuclear Structure II

Project Manager
Dr. Marco Knöll

Researchers
Dr. Julius Müller, Tobias Wolfgruber and Vanessa Neumann

Principal Investigator
Prof. Dr. Robert Roth

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Clusters
Lichtenberg II Cluster Darmstadt

Additional Software
COCONUT

Institute
Institut für Kernphysik

University
Technische Universität Darmstadt

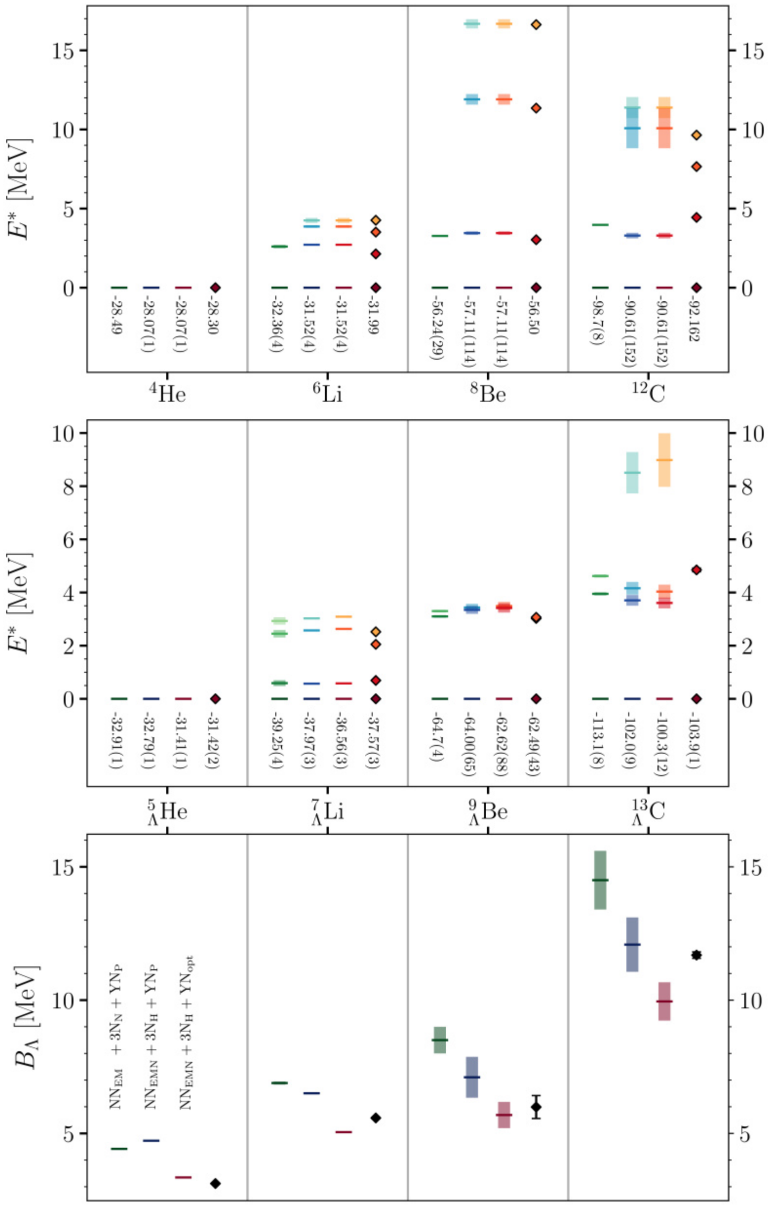

Figure 1: A recent study of extrapolated excitation spectra and hyperon separation energies of the low-lying natural-parity states for selected hypernuclei (middle and lower panels) and their parent nuclei (upper panel) obtained with the IT-NCSM, alongside experimental values (), showing the dependence of hypernuclear observables on the employed NN+3N interactions (left and middle columns for each nucleus) and the improved description through an optimization of LECs in the YN interaction at LO based on p-shell hypernuclei (right columns). The results are accompanied by uncertainties obtained with novel machine learning techniques.

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

The methodological back-bone of the research project is the Importance-Truncated No-Core Shell Model (IT-NCSM), one of the modern ab initio manybody methods that was developed in our group. It provides quasi-exact solutions of the many-body Schrödinger equation for nuclei, a large-scale eigenvalue problem, up to mass $A \approx 25$ 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. Recent extensions of the method allow for calculations of nuclear resonances and hypernuclei. In order to overcome the limitations of the IT-NCSM due to rapidly growing modelspace dimensions we further employ artificial neural networks to predict solutions in infinite model-spaces from series of calculations in finite model-spaces, thus, extending the reach of the method and providing a reliable uncertainty measure for our calculations.

Results

We have performed ab initio NCSM calculation for light to mid-p-shell (hyper)nuclei focusing on different aspects: The first aspect was the development and validation of new families of nuclear interactions from chiral effective field theory with different chiral orders to allow of a systematic quantification of theory uncertainties due to the truncation of the chiral expansion. We have explored this uncertainty quantification for NCSM calculations using semi-local interactions and developed new Bayesian schemes for correlated observables. Similarly, we have developed and studied an optimized hyperon-nucleon interaction, which is constrained on p-shell hypernuclear observables in addition to the very limited hyperon-nucleon scattering data available. A second aspect was the focus on NCSM calculations of charge radii and the development of new tool to improve the precision of NCSM predictions and to asses uncertainties resulting from incomplete model-space convergences. Based on a huge set of training data this machine learning tool is able to provide extrapolations of NCSM calculations for binding energies, excitation energies, hyperon separation energies and radii to infinite model spaces along with a statistical uncertainty measure. In addition we have started to explore new single-particle basis sets with an improved long-range behavior as radii are particularly sensitive to this long-range behavior. Finally, we have extended the NCSM by including continuum physics using a Gamov basis and have successfully applied it to nuclear resonances in light hydrogen, helium and lithium isotopes.

Discussion

Our results demonstrate that the IT-NCSM is to day one of the most powerful and versatile ab initio methods for nuclear structure calculations up to p-shell nuclei. We have shown that spectra and radii in p-shell nuclei are well reproduced by nonlocal and semilocal NN+3N chiral interactions within theoretical uncertainties, which we were able to provide through chiral order-by-order calculations. In the hypernuclear regime we were able to show the great potential of introducing observables from p-shell hypernuclei as additional constraints to the poorly constrained hyperon-nucleon interaction. This way we were able to significantly improve the description of spectra in light hypernuclei. However, we have also seen the limitations of a leading-order interaction, which is why there is an apparent need for more work along those lines. The newly developed machine learning tool allows us to extend the reach of the NCSM through a reliable and robust extrapolation from finite to infinite model spaces. It, moreover, provides an uncertainty measure that can consistently estimate many-body uncertainties for ground-state energies, excitation and radii, which is a unique feature of this approach. With many-body uncertainties under control we were able to clearly identify the truncation of the chiral expansion as the main source of uncertainty. However, since interaction uncertainties cannot be addressed in hypernuclei with a leading order interaction these many-body error estimations are of great importance for theoretical predictions of hyperon separation energies. Follow-up projects will focus on extensions of the machine learning tool to other observables. Finally, with the extension to resonance states we have demonstrated the versatility of the NCSM approach, paving the way to future applications beyond bound states allowing us to tackle questions such as the existence of the tetraneutron.

Publications

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