Hessisches Kompetenzzentrum
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Large-Scale Configuration Interaction for Ab Initio Nuclear Structure III

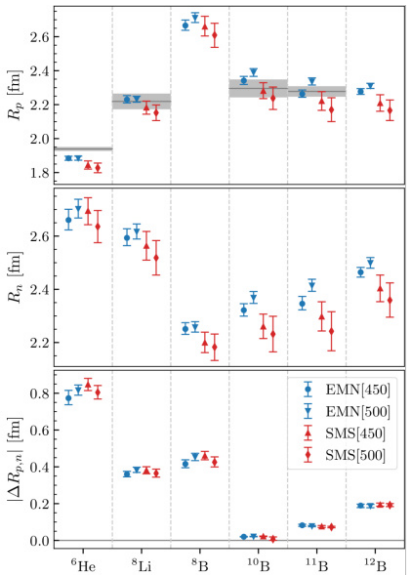


Figure 1: Point-proton radii, point-neutron radii, and radius differences for selected p-shell nuclei obtained with nonlocal (EMN) and semilocal (SMS) chiral two plus three-nucleon interactions at highest chiral order available for cutoffs 450 and 500 MeV. The results are obtained with no-core shell model calculations, which have additionally been extrapolated with artificial neural networks. Error bars account for combined many-body and chiral interaction uncertainties based on statistical estimates and chiral order-by-order analyses. The gray areas represent experimental values with their uncertainties.

Introduction

The prime goal of ab initio (hyper)nuclear structure theory is the description of correlated systems of many baryons based on the fundamental theory of the strong interaction, Quantum Chromodynamics. The quantum many-body problem of the nucleus is especially hard to solve due to the properties of the (hyper)nuclear interaction and range of particle numbers (from 2 to ~300) that is of interest. The methodological backbone of this work is the no-core shell model (NCSM), which 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. Together with supplemental machine learning extrapolation tools that extend the reach of the NCSM and provide uncertainty measures this enables precision studies of energy spectra, radii, and electromagnetic moments and transition strengths in light (hyper)nuclei that are crucial in the effort to refine our understanding of the strong interaction.

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Project Term
2023 - 2024

Clusters
Lichtenberg II Cluster Darmstadt

Additional Software
COCONUT

Institute
Institut für Kernphysik

University
Technische Universität Darmstadt

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Methods

In the NCSM, the quantum many-body problem is cast into the form of a large-scale eigenvalue problem with linear matrix dimensions easily reaching up to 1010. The recent extension to hypernuclei and the consideration of additional particle species further increases the matrix dimension. The computation and storage of the many-body matrix elements and the extraction of low-lying eigenvalues and eigenvectors is a clear HPC challenge and benefits strongly from the hardware setup of Lichtenberg II with its comparatively large main memory per node. In addition to these large-scale memory bound calculations, we have developed machine learning applications based on artificial neural networks that breach the limitations imposed by model-space truncations and enable statistical uncertainty quantification. This requires the training of several thousand neural networks, which is greatly accelerated through parallelization capabilities on the Lichtenberg II cluster.

Results

Throughout this project we have performed a large number of NCSM calculations of energies, radii, and electromagnetic moments for a wide range of p-shell (hyper)nuclei based on the newest generations of realistic interactions from chiral effective field theory at all chiral orders currently available. For the postprocessing of these computations we have refined our machine learning extrapolation framework that extrapolates results in finite model-spaces to the solution in the full Hilbert space and have developed an extension to electromagnetic observables that leverages the correlations between different observables. We have further developed a complete uncertainty quantification that combines statistical many-body uncertainty estimates for the truncation of the model space with interaction uncertainties for the truncation of the chiral expansion obtained in a Bayesian manner. Based on these tools, we have performed precision studies of mass radii and point-proton radii in boron isotopes and electric quadrupole moments across the p-shell. Beyond these efforts in the nuclear regime, we have investigated a newly developed hyperon-nucleon interaction across the ${}_{\Lambda}$He and ${}_{\Lambda}$Li isotopic chain. We have further extended the concept of natural orbitals as a single-particle basis to include hyperons and investigated halo phenomena in different p-shell hypernuclei based on the structural information this basis holds.

Discussion

Our work has demonstrated that machine-learning applications enable the NCSM to reach a high-level of precision for the full suite of nuclear observables. Our detailed studies of different interaction models have been performed in close collaboration with experiment, as our framework also allows the calculation of differences of radii, that directly relate to properties measured in current experiments. These combined efforts enable unique insights into the details of the strong interaction as the present level of precision now allows for a systematic comparison with

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experiment across a wide range of nuclei and observables. The developments in the hypernuclear sector have shown that the new hyperon-nucleon interactions constrained on structure data from p-shell hypernuclei can lift the systematic overbinding of the hyperon. Further, the natural orbital basis does not only provide insights into the structural composition of hypernuclei but also paves the way towards ab initio calculations of medium-mass hypernuclei.

Publications

Knöll, M.; Roth, R.: "Hyperon-nucleon interaction constrained on light hypernuclei", Phys. Lett. B 846, 138258 (2023) https://doi.org/10.1016/j.physletb.2023.138258

Wolfgruber, T.; Knöll, M.; Roth, R.: "Precise neural network predictions of energies and radii from the no-core shell model", Phys. Rev. C 110, 014327 (2024) https://doi.org/10.1103/PhysRevC.110.014327

Knöll, M.; Roth, R.: "Halo structures in p-shell hypernuclei with natural orbitals", arXiv 2501.08013 (2025) https://doi.org/10.48550/arXiv.2501.08013

Knöll, M.; Agel,M. L.; Wolfgruber, T.; Maris, P.; Roth, R.: "Machine learning for correlations of electromagnetic properties in ab initio calculations", arXiv 2501.08959 (2025) https://doi.org/10.48550/arXiv.2501.08959

Marco Knöll; Doctoral Thesis: "Ab initio theory and machine learning for hypernuclei"; TU Darmstadt https://doi.org/10.26083/tuprints-00027654

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