Fully Open-Shell Medium-Mass Nuclei and Electromagnetic Observables for Ab Initio Nuclear Structure IV

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Clusters
Lichtenberg II Cluster Darmstadt

Additional Software
COCONUT

Institute
Institut für Kernphysik

University
Technische Universität Darmstadt

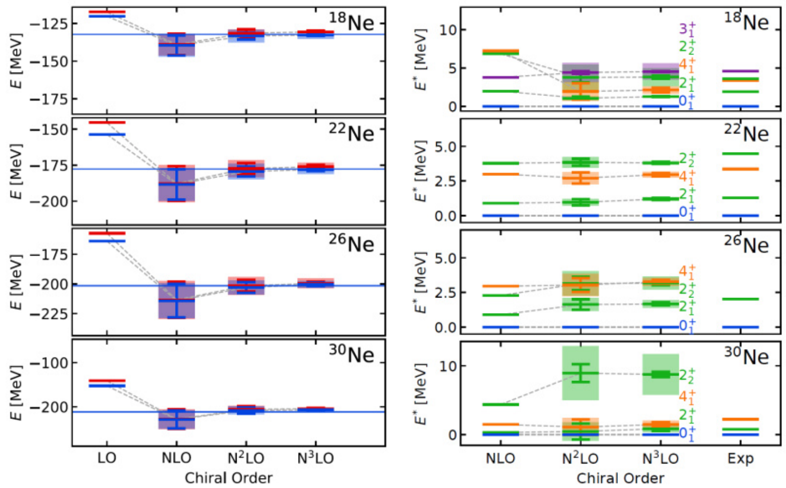

Figure 1: Ground-state energies (left column) and excitation spectra (right column) of selected neon isotopes obtained with nonlocal chiral two plus three-nucleon interactions up to next-to-next-to-next-toleading order of the chiral expansion. The order-by-order dependence of observables is used to quantify the theory uncertainties resulting from the Hamiltonian (bars) and different model-space truncations are used to quantify the many-body uncertainties (bands).

Introduction

The ab initio description of medium-mass nuclei is one of the most dynamic frontiers in nuclear structure theory. One many-body approach in particular, the In-Medium Similarity Renormalization Group, has become a powerful and flexible tool for the description of the full portfolio of nuclear structure observables. In this framework, we have developed the In-Medium No-Core Shell Model, which provides access to ground and exited-state observables of closed and open-shell nuclei up into the intermediate mass regime. This allows us to connect the underlying physics of the strong interaction, captured in chiral effective field theory, with nuclear structure observables in the regime of stable and exotic nuclei that are being studied experimentally at several labs worldwide, including FAIR/GSI.

Methods

For studying a broad range of open-shell medium-mass nuclei, we have developed a novel hybrid ab initio method, the In-

Medium No-Core Shell Model (IM-NCSM). This method builds on the flexibility of the No-Core Shell Model and supplements it with a multi-reference formulation of the In-Medium Similarity Renormalization Group (IM-SRG) decoupling of the underlying Hamiltonian. In this way, the convergence of the NCSM is drastically enhanced, so that arbitrary closed and open-shell nuclei in the medium-mass domain become accessible. The IM-NCSM provides access to the full range of nuclear structure observables, including electromagnetic transition strengths and moments that define nuclear spectroscopy and that are of particular interest in connection with ongoing experiments. The study of these observables is at the heart of the research program of our research group. The computational methods used in the IM-NCSM, which include the solution of initial value problems of systems of $\sim 10^6$ coupled differential equations as well as sparse matrix eigenvalue problems with linear matrix dimensions of up to 10^8, rely on highperformance computers and benefit strongly from the hardware setup of Lichtenberg II with its comparatively large main memory per node. Without such an HPC system our studies would not have been possible.

Results

We have focused on the characterization and application of new families of chiral two plus three-nucleon interactions form chiral effective field theory. We have explored two specific families of interactions with different regulator schemes, nonlocal and semilocal regulators, and a range of chiral truncations from leading order to next-to-next-to-next-toleading order and beyond. This enables a systematic quantification of the theory uncertainties resulting from the truncation of the chiral expansion using sophisticated Bayesian methods. Furthermore, the control over all relevant truncations of the many-body model space enables the quantification of the many-body truncation uncertainties. Although this explicit uncertainty quantification increases the computational cost by about one orderof-magnitude, it is vital for confronting ab initio predictions of nuclear observables with experiment. We have explored this scheme based on the IM-NCSM for several mediummass nuclei, mainly in the oxygen, neon, and magnesium isotopic chains from stable isotopes to the driplines. We have focused on ground-state and excitation energies, charge radii, and low-lying and collective transition strengths. The latter includes an additional methodological development, where we replace the NCSM diagonalization with an equations-of-motion method. Among the highlight publications resulting from this project are two joint papers with experimental groups on charge radii in nickel isotopes, two papers on collective excitations in medium-mass nuclei, and one comprehensive paper with the LENPIC collaboration on the latest results with semilocal interactions and advanced Bayesian uncertainty quantification schemes.

Discussion

Our studies demonstrate the predictive power of modern ab initio methods based on chiral effective theory inputs, but they also reveal some deficiencies that will be the subject of future investigations. We have shown that nonlocal NN+3N interactions allow for a robust prediction of ground-state and excitation energies in the p and sd-shell which agree with experiment within the theoretical uncertainties. Also charge radii are well reproduced with the nonlocal family of chiral interactions. For semilocal interactions, however, we observe a significant underestimation of charge radii beyond the light nuclei, although ground-state energies are still in good agreement with experiment. Since we have full control over the many-body uncertainties in the IM-NCSM, we can clearly identify the chiral inputs as origin of this discrepancy. Such regulator-scheme dependencies of selected nuclear observables are unexpected and will be analyzed in more detail in future studies. Furthermore, our studies also reveal limitations of the IM-SRG framework itself. Particularly for electric quadrupole observables, we observe increased many-body uncertainties for specific isotopes. In these cases, the reference states used for the multi-reference IM-SRG decoupling are missing important static correlations. Based on these observations we are planning to extend the IM-NCSM framework to allow for a more flexible refence-space truncation. We will develop an active-space configuration interaction approach combined with the multi-reference IM-SRG to capture important static correlations from the outset. This follow-up project will be a central part of our research activities in the third funding period of the DFB SFB 1245.

Publications

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