Hessisches Kompetenzzentrum für Hochleistungsrechnen

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

Project Manager
Tobias Mongelli

Researchers
Laura Mertes and Carl Walde

Principal Investigator
Prof. Dr. Robert Roth

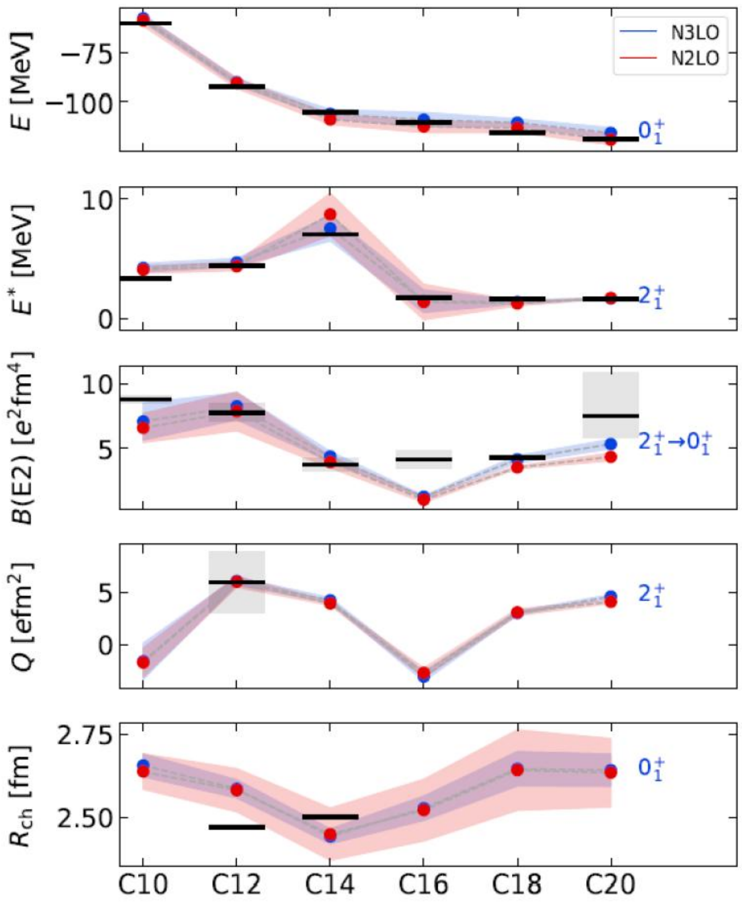
Project Term
2020 - 2021

Clusters
Lichtenberg Cluster Darmstadt

Additional Software
COCONUT

Institute
Institut für Kernphysik

University
Technische Universität Darmstadt



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

Introduction

The ab initio description of nuclear structure phenomena has progressed tremendously over the past years. In particular, the recent development and extension of innovative many-body methods for the description of medium-mass systems has emerged as a pillar of modern theoretical nuclear structure physics, which allows for systematically improvable, approximate solutions of the time-independent Schrödinger equation.
However, even though being well established, a highly accurate solution requires significant computational resources—the numerical solution of the Schrödinger equation rapidly becomes intractable even on supercomputing facilities. Only the development of new many-body approaches and new algorithms allows us to push the mass frontier towards heavier systems and away from shell closures.
Our research group has developed several novel hybrid many-body methods that allow to address nuclear observables of arbitrary open-shell systems far away from shell closures, which could only partially be described via controlled expansion methods in the past. The most versatile of these hybrid methods is the In-Medium No-Core Shell Model (IM-NCSM), which allows for the description of genuine open-shell nuclei in a no-core ab initio framework.

Methods

For studying a broad range of open-shell medium-mass nuclei, we have developed two novel hybrid ab initio methods, the In-Medium No-Core Shell Model (IM-NCSM) and the perturbatively improved No-Core Shell Model (NCSM-PT). Both methods build on the flexibility of the NCSM and supplement it either with a Multi-Reference In-Medium Similarity Renormalization Group (MR-IM-SRG) decoupling of the underlying Hamiltonian or with an a *posteriori* correction via low-order Multiconfigurational Perturbation Theory. 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. While the NCSM-PT is limited to the description of ground and excited state energies, the IM-NCSM provides access to the full range of nuclear structure observables. This includes electromagnetic transition strengths and moments that define nuclear spectroscopy and are of particular interest in connection with ongoing experiments.
Only recently, we have extended the IM-NCSM to the description of electric quadrupole and magnetic dipole observables, which requires a consistent Magnus transformation of non-scalar operators. The study of these observables will be at the heart of the research program of our research group for the coming years.

Results

Figure 1 shows a summary of the results for the carbon isotopic chain, including electric quadrupole observables and charge radii.

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

The order-by-order convergence of various observables for ^{20}Ne is shown in figure 2 for different truncations N^{ref}_{max} of the reference space. The two types of error bars indicate the interaction and the many-body uncertainties.
We have performed a first proof-of-concept calculation for a leading order three-body correction which is shown in figure 3.

Discussion

We have focused our investigations in the past project period on the characterization and application of new families of chiral two plus three-nucleon interactions. We have explored two specific families of interactions with di erent regulator choices, nonlocal and semilocal regulators. A complete quantification of theory uncertainties is a central goal of modern ab initio nuclear structure theory.
Using these interactions, we have explored the spectroscopy of carbon isotopes from ^{10}C to ^{20}C. These calculations not only address ground-state energies and radii, but also excitation spectra and electromagnetic transitions and moments. Further, we have extended the In-Medium NCSM to the use of consistently free-space SRG-evolved electric quadrupole and magnetic dipole operators. Furthermore, we have started to explore the neon isotopic chain, employing the same family of chiral interactions. For this isotopic chain we computed ground state energies, spectra, electromagnetic moments and transition strengths and charge radii and we explore the predicted position of neutron dripline in comparison to experimental data.
Finally, we have developed a leading-order three-body correction for the MR-IM-SRG(2) for scalar and non-scalar operators in the m-scheme, since the full treatment of three-body interactions is computational very expensive and not feasible at the moment. Using this correction we have performed a first proof-of-concept calculations and showed that the influence on the ground- and excited state energies is small.

Figures

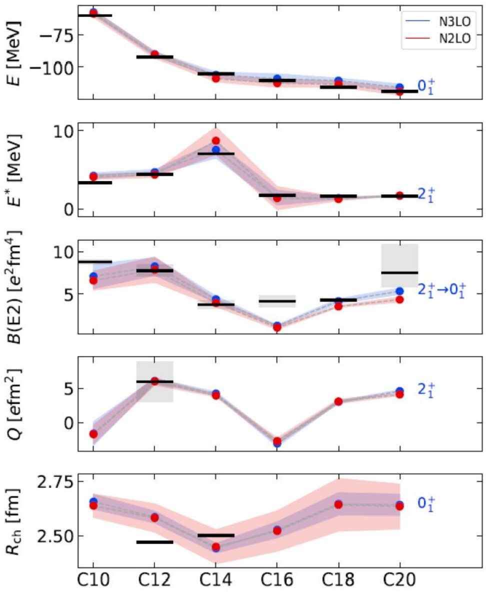


Figure 1: Scalar and non-scalar observables for di erent carbon isotopes with combined interaction and many-body uncertainties.

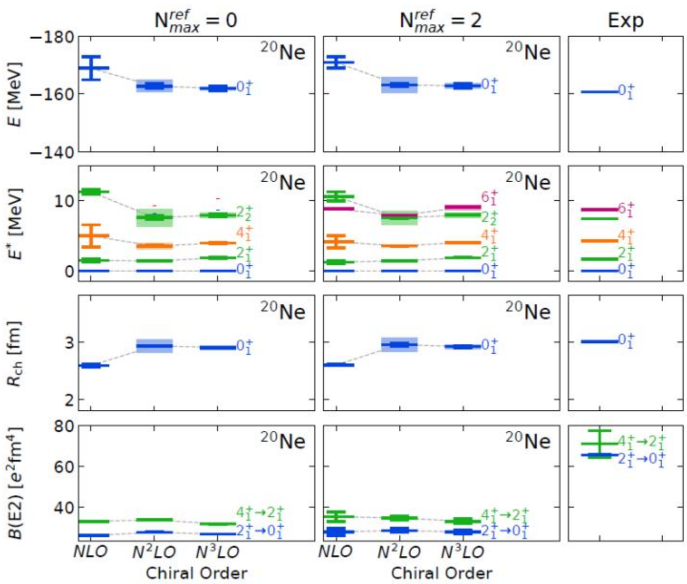


Figure 2: Scalar and non-scalar observables for ^{20}Ne with interaction and many-body uncertainties.

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

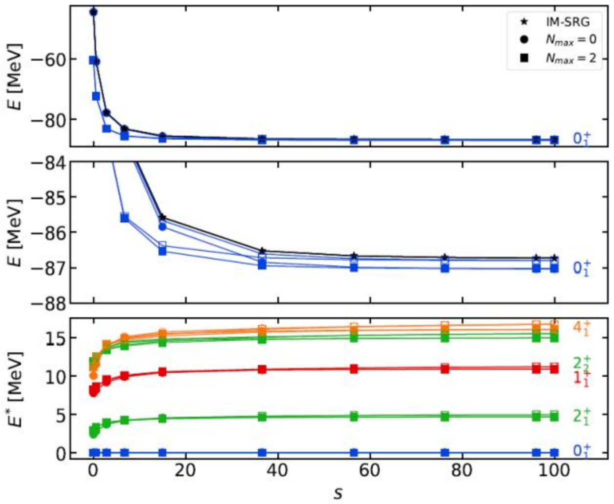


Figure 3: Ground-state energy and spectrum plotted as function of the flow parameter *s* for ^{12}C, where the induced three-body correction is compared to the NO2B approximation.

Publications

Friman-Gayer, U.; Romig, C.; Hüther, T. et al.: Role of chiral two-body currents in 6-Li magnetic properties in light of a new precision measurement with the relative self-absorption technique, Phys. Rev. Lett. 126, 102501, 2021
https://doi.org/10.1103/PhysRevLett.126.102501

D'Alessio, A.; Mongelli, T.; Pietralla, N.; Roth, R. et al.: Precision measurement of the B(E2) strength of the 2+ 1 State in ^{12}C, Phys. Rev. C 102, 011302(R), 2020 https://doi.org/10.1103/PhysRevC.102.011302

Tichai, A.; Roth, R.; Duguet, T.: Many-Body Perturbation Theories for Finite Nuclei, Frontiers in Physics 8, 164, 2020
https://doi.org/10.3389/fphy.2020.00164

Heil, S.; Petri, M.; Vobig, K.; Bazin, D. et al.: Electromagnetic properties of 21O for benchmarking nuclear Hamiltonians, Phys. Lett. B 809, 135678, 2020 https://doi.org/10.1016/j.physletb.2020.135678

Hüther, T.; Vobig, K.; Hebeler, K.; Machleidt, R.; Roth, R.: Family of Chiral Two- plus Three-Nucleon Interactions for Accurate Nuclear Structure Studies, Phys. Lett. B 808, 135651, 2020
https://doi.org/10.1016/j.physletb.2020.135651

Last Update: 2022-04-05 12:36