Hessisches Kompetenzzentrum
für Hochleistungsrechnen

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



Project Manager
Klaus Vobig

Principal Investigator
Prof. Dr. Robert Roth

Project Term
2018 - 2019

Project Areas
Particles, Nuclei and Fields

Institute
Institut für Kernphysik

University
Technische Universität Darmstadt

Introduction

The ab initio description of nuclear physics 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 allow for systematically improvable, approximate solution of the time-independent Schrödinger equation. The use of such expansion methods for the solution of the quantum many-body problem beyond the carbon chain has become a standard tool by now.

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. This opens up a vast territory of new nuclear structure predictions, which previously were out of reach for ab initio methods.

Methods

For studying a broad range of fully open-shell medium-mass nuclei we employed two novel NCSM-based medium-mass

methods, the In-Medium No-Core Shell Model (IM-NCSM) and the perturbatively improved No-Core Shell Model (NCSM-PT), which allow for the description of arbitrary open-shell nuclei in an ab initio framework. Both methods o er great flexibility in accessing diverse nuclear structure observables for a broad range of nuclei which makes our approaches unique in the ab initio community. In particular both methods tremendously extend the reach of no-core approaches and allow for the calculation of nuclear observables at only a fraction of the computational costs of large-scale NCSM calculations.

Results

In the IM-NCSM in-medium correlations are summed into a similarity-transformed Hamiltonian via using the multi-reference IM-SRG flow equations and a subsequent diagonalization giving access to ground and excited states of medium-mass nuclei. Applications to neutron-rich carbon and oxygen isotopes showed excellent agreement with large-scale NCSM calculations [1]. Furthermore, we eliminated the restriction to even nuclei of the IMNCSM via a particle-attached/particle-removed extension of the IM-NCSM. By implementing the consistent transformation of non-scalar sperical tensor operators with the MR-IM-SRG, we are now in the position to employ the IM-NCSM for the of study electromagnetic observables. This opens up the possibility to fully explore nuclear structure of all nuclei in the medium-mass range including the study of, e.g., island-of-inversion physics like the exploratory study of two selected magnesium isotopes.

Discussion

The NCSM-PT follows a diagonalize-then-perturb philosophy, where NCSM eigenvectors of limited size are taken as zero-order input for a multi-configurational version of MBPT. Merging NCSM with MBPT allows for keeping the advantages of both methods while overcoming their individual limitations. NCSM on the one hand is a fully variational method which is limited by its exponential scaling to light nuclei. MBPT on the other hand e ectively incorporates dynamic correlations from large model spaces. Combining both approaches significantly extends the reach of NCSM-based methods via a perturbative treatment of residual correlation e ects beyond the zero-order reference space. We applied second-order NCSM-PT to carbon, oxygen and fluorine isotopic chains and compared our results to large-scale diagonalizations.

Outlook

The very good agreement of the calculated ground-state and excitation energies shows great promise for future applications beyond the lower sd-shell [2]. Due to its low computational cost and its high accuracy, the NCSM-PT is the ideal tool to meet the ongoing requirement for exploratory studies of new generations of chiral interactions over a large range of nuclei.

JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN TECHNISCHE UNIVERSITÄT DARMSTADT UNIKASSEL VERSITÄT Philipps Universität Marburg

Reference

[1] Gebrerufael, E., Vobig, K., Hergert, H., Roth, R.: "Ab Initio Description of Open-Shell Nuclei: Merging No-Core Shell Model and In-Medium Similarity Renormalization Group", Phys. Rev. Lett. 118, 152503, (2017). https://doi.org/10.1103/PhysRevLett.118.152503

[2] A. Tichai, E. Gebrerufael, and R. Roth, “Open-Shell Nuclei from No-Core Shell Model with Perturbative Improvement”, submitted for publication in Physical Review Letters (2017). https://doi.org/10.1016/j.physletb.2018.10.029

Last Update: 2022-10-11 11:29