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

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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.

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Reference

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