Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Large-Scale Configuration Interaction for Ab Initio Nuclear Structure

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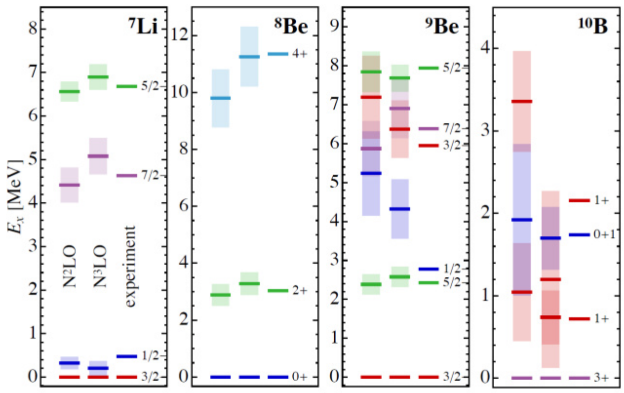
Project Term
2019 - 2020

Clusters
Lichtenberg Cluster Darmstadt

Additional Software
COCONUT, NCSM

Institute
Theoriezentrum Institut für Kernphysik

University
Technische Universität Darmstadt



Introduction

The goal of *ab initio* nuclear structure theory is the description of correlated systems of many nucleons based on the fundamental theory of Quantum Chromodynamics (QCD). We are faced with two challenges: First, the interaction itself is not well-known. Second, the quantum many-body problem of the nucleus is especially hard to solve due to the properties of the nuclear interaction and range of relevant particle numbers. In this project, we cast the quantum many-body problem into the form of a large-scale eigenvalue problem, extract the lowest lying eigenvalues and eigenvectors and from there calculate further observables.

Methods

The research project employs the Importance-Truncated No-Core Shell Model (IT-NCSM), a modern ab initio many-body method. It provides quasi-exact solutions of the many-body Schrödinger equation for nuclei up to mass A ≈ 25. The algorithm is based on a matrix representation of the Hamiltonian and a subsequent solution of the matrix-eigenvalue problem. Each calculation involves three main phases of different computational character: the setup of the importance-truncated basis, the computation of the many-body matrix elements of the observables, and the iterative calculation of low-lying eigenvalues and eigenvectors. The basis dimensions implies a significant amount of aggregated RAM needed for storing the matrices.

Results

Our research goals were the construction of accurate nuclear interactions from chiral effective field theory that enable a consistent and realistic description of nuclear properties, and the support of state-of-the-art experiments by providing precision calculations and predictions for specific nuclei. With a new family of chiral two plus three-nucleon interactions up to next-to-next-to-next-to-leading-order in the chiral expansion and a new fit protocol, we established a scheme which consistently reproduces ground state energies and charge radii from light nuclei up into the medium-mass regime. Since we have systematic interactions for four successive chiral orders and three different cutoffs available, we can apply a rigorous uncertainty quantification scheme, which is an important advance for ab initio nuclear structure theory. We have performed several precision studies of electromagnetic observables in light nuclei, which led to joint experiment-theory publications in high-profile journals. This tied in with the experimental work in the group of Prof. Nörtershäuser was identified as a key research topic in the DFG Collaborative Research Center 1245. We have studied the charge radii of ^{10}B and ^{11}B and a joint publication has appeared in Physical Review Letters and was highlighted in a press release of TU Darmstadt. In another project, we studied the quadrupole moment of the 2^+ state and the B(E2) transition strength from the 2^+ state to the ground state in ^{12}C. These studies complement a new experiment on the B(E2) in the group of Prof. Pietralla. We present the most accurate determinations of these two observables yet, for the quadrupole moment we were able to reduce the uncertainty compared to the present literature value by a factor of 10. This work has been accepted for publication as a Rapid Communication in Physical Review C. In a third project, we have performed precision NCSM calculations of magnetic dipole observables in ^{6}Li. In a joint study with the group of Prof. Pietralla, we have computed the B(M1) transition strength and the magnetic dipole moment including two-body current corrections to the M1 operator from chiral EFT, together with a consistent SRG-evolution of all operators. Both elements were important to get a precise description, which is compatible with the new experimental values within uncertainties. These results have been submitted for publication to Physical Review Letters.

Discussion

Our work during the past project period has demonstrated that high-performance computing is critical to advance our understanding of nuclear structure physics and to unlock the full potential of modern nuclear structure experiments. Only the combination of advanced nuclear theory, driven by innovative computational methods and the availability of resources on high performance computers like Lichtenberg, and new experiments will lead to a comprehensive understanding of the nuclear many-body problem.

Figures

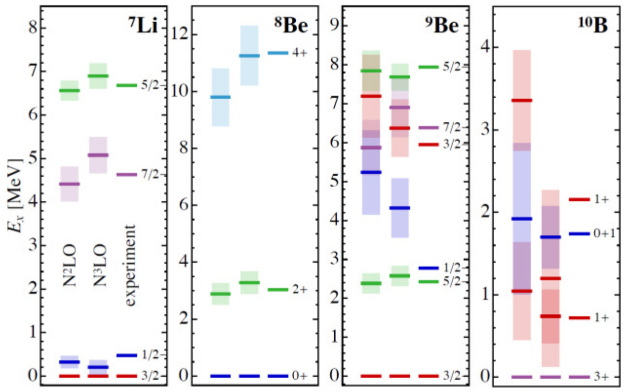


Figure 1: Spectra of selected p-shell nuclei obtained in the NCSM with a new family of two-plus three-nucleon interactions from chiral effective field theory, including a full quantification of theory uncertainties.

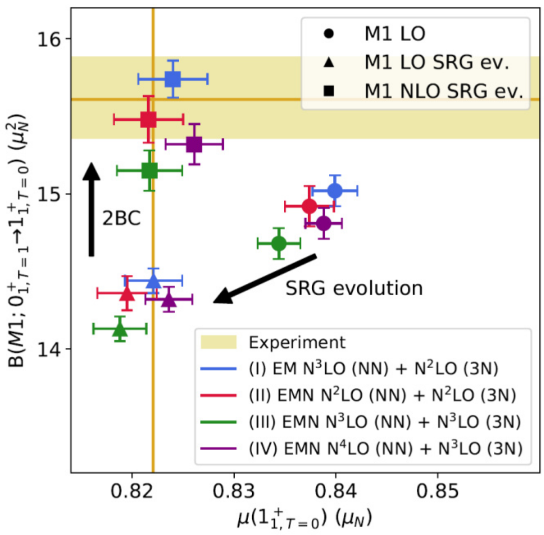


Figure 2: Magnetic dipole observables obtained in the NCSM for 6Li, for di erent chiral two-plus three-nucleon interactions, including two-body current (2BC) corrections to the magnetic dipole operator in comparison to a new precision experiment for the magnetic dipole transition strength.

Publications

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