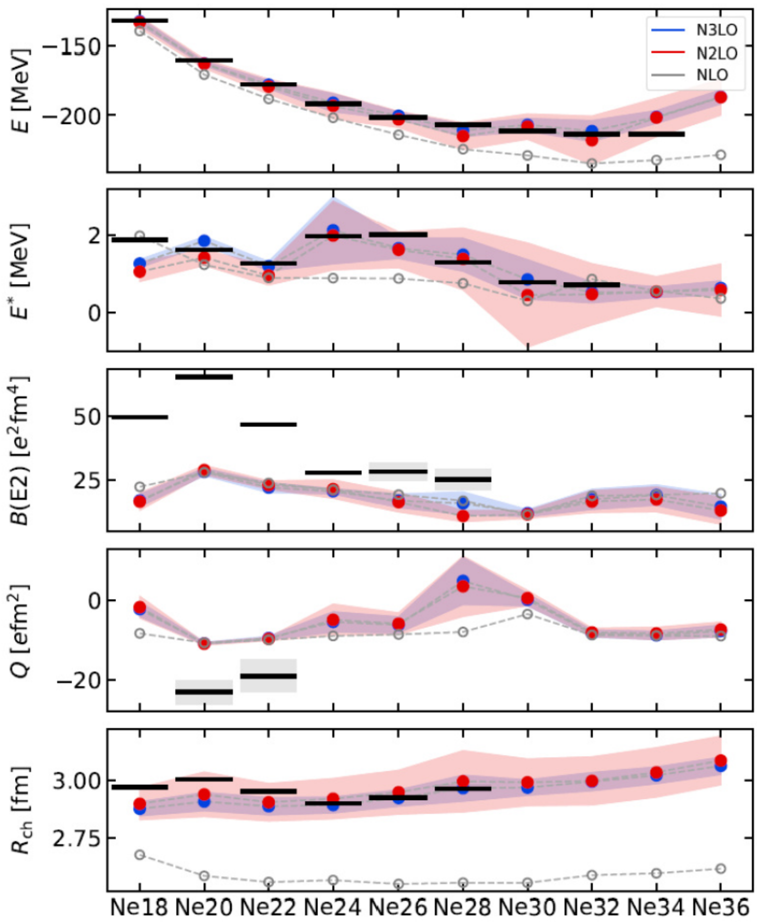
Hessisches Kompetenzzentrum für Hochleistungsrechnen

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



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Project Term
2021 - 2022

Clusters
Lichtenberg Cluster Darmstadt

Additional Software
COCONUT

Institute
Institut für Kernphysik

University
Technische Universität Darmstadt

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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 even isotopes of the neon isotopic chain, including electric quadrupole observables and charge radii as function of the isotope. The error bars indicate combined many-body and interaction uncertainties. The

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order-by-order convergence of magnetic dipole observables for $^{18\text{-}25}Ne$ 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.

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 different 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 neon isotopes from ^{18}Ne to ^{36}Ne. These calculations not only address ground-state energies and radii, but also excitation spectra and electromagnetic transitions and moments using consistently free-space SRG-evolved electric quadrupole and magnetic dipole operators. For the even neon isotopes, the ground-state energies charge radii and first excited-state energies are in good agreement with experimental. For the electric B(E2) transition strengths and quadrupole moments we obtain a systematic underestimation, which could be due to neglected higer-body terms in the IM-SRG evolution. Furthermore, all neon isotopes show deformation or clustering behaviour. It could be that the IM-NCSM does not capture enough of these deformation effects. For the magnetic monopole observables the results agree more with the experimental compared to the electric quadrupole observables. Especially the magnetic dipole moments of $^{20\text{-}22}Ne$ are in good agreement.

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Figures

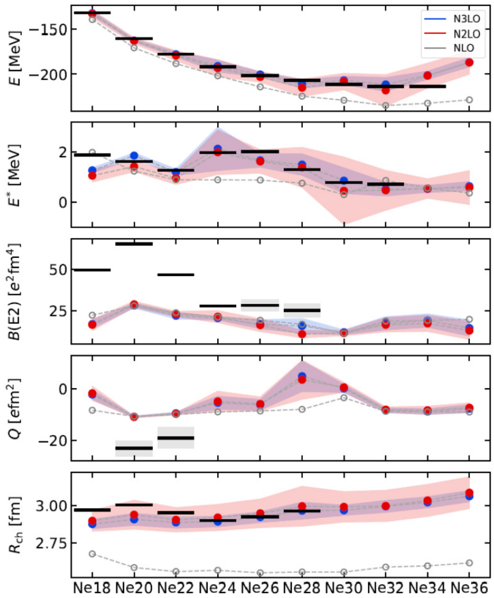

Figure 1: Ground-state energies, first excited-state energies, B(E2) transition strengths, electric quadrupole moments and charge radii for $^{18-36}$Ne as function of the isotope for different chiral orders ranging from NLO to N^{3}LO. The error bands indicate combined many-body and interaction uncertainties.

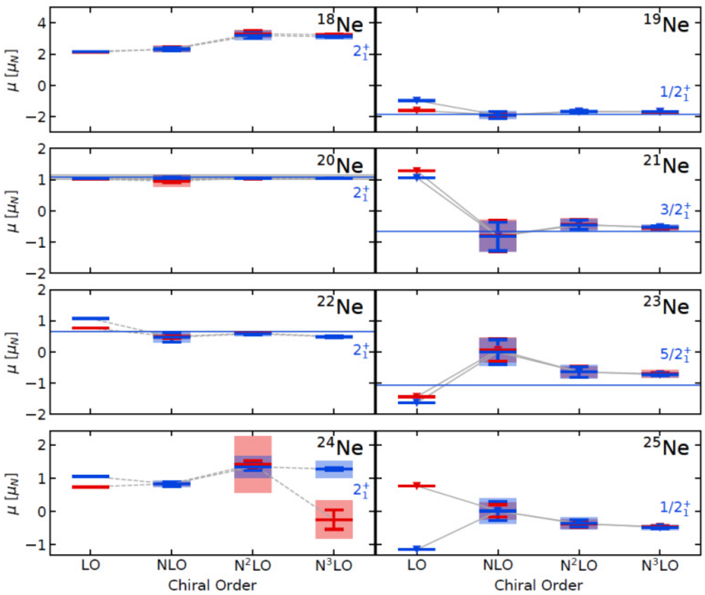

Figure 2: Magnetic dipole moments for different neon isotopes $^{18-25}$Ne as function of the chiral interaction order. Red bars are results for N^{ref}_{max} = 0 and blue bars depict results for N^{ref}_{max}= 2. Error bars are interaction uncertainties and shaded bands indicate combined many-body and interaction uncertainties. The solid lines depict experimental results.

Publications

Frosini, M.; Duguet, T.; Ebran, J-P.; Bally, B.; Hergert, H. et al., “Multi-reference many-body perturbation theory for nuclei III - Ab initio calculations at second order in PGCM-PT”, Eur. Phys. J. A 58, 63 (2022) https://doi.org/10.48550/arXiv.2111.01461

Frosini, M.; Duguet, T.; Ebran, J-P.; Bally, B.; Mongelli, T. et al., “Multi-reference many-body perturbation theory for nuclei II - Ab initio study of neon isotopes via PGCM and IM-NCSM calculations”, Eur. Phys. J. A 58, 63 (2022) https://doi.org/10.48550/arXiv.2111.00797

Mongelli, T.: “The In-Medium No-Core Shell Model as Comprehensive Ab-Initio Tool”, Doctoral Thesis, TU Darmstadt (2022) https://doi.org/10.26083/tuprints-00021671

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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/10.48550/arXiv.2005.07837

Robert Roth. No-Core Shell Model and Beyond. Online Workshop on Wave-Function Methods in Quantum Chemistry and Nuclear Physics, Saclay, France (February 8 - February 20, 2021)

Robert Roth. Towards Accurate Calculations of Medium-Mass Nuclei. Workshop on Progress in Ab Initio Techniques in Nuclear Physics at TRIUMF, Vancouver, CA (March 3 - March 6, 2020)

Tobias Mongelli. Carbon Isotopes from the In-Medium NCSM.Workshop on Progress in Ab Initio Techniques in Nuclear Physics at TRIUMF, Vancouver, CA (March 3 - March 6, 2020)

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