Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Large-Scale Configuration Interaction for (Ab Initio) Nuclear Structure



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Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas

Clusters
Lichtenberg Cluster Darmstadt

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Introduction

The prime goal of ab initio nuclear structure theory is the description of strongly interacting systems starting from Quantum Chromodynamics (QCD), the theory of the strong interaction. On this path, we are faced with two challenges: the first one is that, unlike e.g. in atomic physics, the interaction itself is not well-known because it cannot be derived directly from QCD. The second one is that the quantum many-body problem is especially hard to solve due to the properties of the nuclear interaction. While this project focuses on the latter challenge, its results provides valuable feedback on the quality of interactions, supporting efforts tackling the first one. In this project period, we have investigated the systematics in electric multipole strength distributions throughout the oxygen isotopic chain. Our approach provides access to the low-energy strength as well as the giant resonance region including fragmentation and fine structure in an ab initio framework. When moving from closed- to mid-shell nuclei, the giant resonance broadens and pygmy dipole excitations emerge. This behavior is compatible with experimental observations. Based on the appearance of strong contributions from low-energyneutron-dominated 2^+ excitations in the isoscalar E2 strength distributions, we predict also a pygmy quadrupole resonance for oxygen isotopes with neutron excess. The existence of such a pygmy quadrupole resonance has been proposed recently and has been confirmed for ^{124}Sn only two years ago. Furthermore, these dynamic observables provide a unique testing ground for nuclear interactions beyond the traditionally used static properties, such as binding energies or radii. Indeed, the calculated strength distributions are located at too high energies, indicating that other aspects of the interaction, e.g., momentum dependencies or non-localities, play an important role for transition strengths. Thus, the availability of this new class of observables in an *ab initio* treatment can provide vital guidance for devising improved interactions in the future.

Methods

In the low-mass regime, we have calculated the four neutron system and the possible location of a low-lying resonance within the scope of the Harmonic-Oscillator Representation of Scattering Equations (HORSE) method. We studied a broad variety of state-of-the-art nuclear interaction and their effect on the existence and corresponding location and width of a 4n resonance. We could show that, at least within the used method, the existence and gross propertiesof a 4n resonance do not depend on the choice of interaction. These results, in combination with the veri- or falsification by experiment of the 4n resonance in the coming years, will deliver important feedback to the quality of nuclear interactions. In the project part involving strangeness degrees of freedom, we calculated ground-state and hyperon-separation energies of medium-mass hypernuclei with closed nucleonic cores using the Hartree-Fock method, second-order many-body perturbation theory, and the Brueckner-Hartree-Fock approximation. These calculations are the first of their kind employing similarity-renormalization-group

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evolved chiral Hamiltonians and including induced hyperon-nucleon-nucleon interactions.

Results

By comparing our results to results from quantum monte-carlo calculations and to an empirical mass formula, we could confirm the importance of the induced hyperon-nucleon-nucleon terms for the description of hyperon-separation energies of medium-mass nuclei. We also found indications that their inclusion could stiffen the equation of state of neutron-star matter by delaying the appearance of hyperons to higher densities. High performance computing is crucial for all of these advances because the tackled problem sizes are far beyond what a single computer can handle.

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