Subproject D1: Theoretical Nuclear Structure Physics

Nuclear theory has entered an exciting era of structure and reaction calculations connected to Quantum Chromodynamics (QCD) through chiral effective field theory. This is driven by a number of developments ranging from effective field theory, renormalization group (RG), and unitary transformation methods for nuclear forces to powerful ab-initio and approximate many-body methods including the application of large-scale computing resources. Significant progress on these fronts has been made in the previous funding periods. The aim of project D1 is to further advance these innovative methods to a systematic description of structure and reaction calculations for a range of nuclei and observables based on chiral effective field theory interactions. The focus lies on the development and application of microscopic many-body approaches including three-nucleon (3N) interactions based on chiral effective field theory, with specific attention to the experimental studies in project areas A, B and C.

The main aspects of our ongoing research are listed below:

**Consistent unitary transformations of chiral NN plus 3N interactions**

To facilitate the solution of the many-body problem, i.e., to improve the convergence of the results as function of model-space size, we can use unitary transformations to soften or pre-diagonalize the Hamiltonian. We have developed and studied these unitary transformations extensively at the two-body level, e.g., in the framework of the Unitary Correlation Operator Method (UCOM) or the Similarity Renormalization Group (SRG). Now, we extend these transformations to the three-nucleon sector, thus providing consistent unitarily-transformed NN plus 3N Hamiltonians starting from chiral NN at next-to-next-to-next-to (N^3LO) plus 3N at next-to-next-to (N^2LO) interactions, respectively. These transformed Hamiltonians and the corresponding transformed operator serve as input for a broad range of nuclear structure calculations in projects D1 and D2.N3LO

Initially, we will focus on the SRG transformation in a matrix representation in three-body space. Although conceptually straightforward, the computation and handling of the three-body matrix elements are challenging. We carry out the transformation in three-body space, using Jacobi-coordinate harmonic-oscillator matrix elements for the SRG evolution and a subsequent transformation to JT-coupled matrix elements entering into the many-body calculations. We will refine and optimize this scheme to eventually compute and handle all 3N matrix elements needed, e.g., for 14ℏΩ No-Core Shell Model (NCSM) calculations of all p-shell nuclei.

In this framework we will study several important aspects of the SRG transformation, mainly regarding the convergence properties of the resulting Hamiltonians and the size of the induced 3N and 4N interactions. We will investigate different forms of the SRG generator aiming to optimize convergence and to minimize induced many-body contributions. We will consider consistent SRG-evolutions of various other observables and study their sensitivity to the transformation and to short-range correlations.

Once available in terms of matrix elements, we will start to extend these investigations to chiral 3N interactions at N^3LO and possibly 4N contributions. We will include the dominant
terms of the N$^3$LO chiral 3N interactions, guided by the nuclear-matter studies within this project (see below), into our matrix-element calculation and study the sensitivity of the Hamiltonian and of selected many-body calculations on these terms.

**In-Medium Similarity Renormalization Group for nuclei**

With K. Tsukiyama and S.K. Bogner, we have developed a new ab-initio method that uses the SRG to continuously diagonalize nuclear many-body Hamiltonians. In contrast to applications of the SRG to NN and 3N interactions in free space, we have applied the SRG evolution “in-medium” directly in the A-body system of interest. The In-Medium Similarity Renormalization Group (IM-SRG) approach has the advantage that one can approximately evolve 3,...,A-body operators using only two-body machinery based on normal-ordering techniques. The method can be tailored to a variety of problems ranging from the diagonalization of closed-shell nuclei to the construction of effective valence shell-model Hamiltonians and operators. We have obtained first very promising results for the ground-state energies of $^4$He, $^{16}$O and $^{40}$Ca for NN forces, with accuracies comparable to Coupled-Cluster (CC) calculations.

We will extend the IM-SRG to include 3N forces, first for the ground-state energies of the doubly-magic nuclei $^4$He, $^{16}$O and $^{40}$Ca at the normal-ordered two-body level. We will explore the connections of the IM-SRG and CC theory, and use CC and NCSM/IT-NCSM calculations to benchmark the IM-SRG results for medium-mass nuclei. The IM-SRG evolution is already set up with an efficient parallel J-coupled code, thus making it possible to include full normal-ordered three-body contributions, especially if required by the comparison with CC calculations. In addition, we will apply the IM-SRG to derive valence-nucleon interactions in the sd- and pf-shell and to consistently evolve electroweak operators. The IM-SRG derivation of valence-nucleon interactions has two key advantages over present approaches to effective shell-model Hamiltonians: it is nonperturbative and treats the particle-particle/hole-hole and particle-hole channels on an equal footing; and it can also be applied to derive cross-shell interactions, which are treated very phenomenologically in present structure calculations. A milestone application of the IM-SRG operator evolution will be to neutrinoless double-beta decay nuclear matrix elements. The IM-SRG developments will be carried out in collaboration with S.K. Bogner (MSU/NSCL).
Ab-initio spectroscopy of p- and sd-shell nuclei with transformed NN plus 3N interactions

Using SRG-transformed NN plus 3N interactions, we will investigate the structure and spectroscopy of nuclei throughout the p-shell and the lower sd-shell. For the ab-initio solution of the many-body problem we will mainly use the Importance-Truncated No-Core Shell Model (IT-NCSM) which we developed in the previous funding periods. It enables us to include 3N interactions without approximation for model spaces beyond the reach of any present NCSM code. Due to the importance truncating scheme and the JT-coupled scheme of the three-body matrix elements we are able to perform calculations using complete SRG-transformed chiral NN plus 3N interactions for nuclei like $^{10}$B, $^{12}$C or $^{16}$O in up to $14\hbar\Omega$ model spaces. For soft SRG-transformed interactions this will be sufficient to warrant convergence of the spectrum. We have demonstrated the feasibility of these calculations in several recent pilot runs using a first version of the IT-NCSM code including explicit 3N interactions. In this funding period we will further improve the IT-NCSM scheme and the handling of 3N matrix elements.

These studies have two complementary aims: On the one hand, the ground states and excitation spectra of light nuclei provide a critical test bed for the chiral NN plus 3N interactions and the SRG transformation. We will analyze the sensitivity of the spectra on the low-energy constants $c_D$ and $c_E$ of the chiral N$^2$LO three-body forces and we will assess the impact of 4N terms induced by the SRG transformation. In addition to a general validation of the approach, this investigation will provide a feedback for the development of chiral EFT interactions based on nuclear structure observables beyond the few-body domain, e.g., regarding the influence of higher-order 3N and possibly 4N contributions. This analysis
will also be vital to assess and compare different unitary transformations, i.e., different choices of the SRG generators.

On the other hand, these studies give access to a number of intriguing nuclear structure phenomena that are sensitive to 3N interactions and have not been understood quantitatively so far. We will study the spectra and spectroscopic observables for p-shell isotopes of interest for the experimental program, e.g., the properties of the first $1/2^+$ state in $^9\text{Be}$ that was studied in project A2. We will investigate the systematics of $2^+$ excitation energies and $B(E2)$ transition strengths in the carbon isotopic chain up to the neutron drip line. Recent controversial measurements indicate an anomalous deviation of the $B(E2)$ in $^{16}\text{C}$ from the general systematics which is not understood so far. The IT-NCSM is one of the few methods that can address these questions in an ab-initio sense starting from consistently SRG-evolved chiral NN plus 3N interactions.

**Three-nucleon forces and two-body current operators in the shell model**

Our pioneering extensions to larger nuclei in the shell model have revealed new facets of 3N forces, such as its role in determining the location of the neutron drip line in oxygen and for the doubly-magic nature of $^{48}\text{Ca}$.

With collaborators J.D. Holt (ORNL/UT) and T. Otsuka (Tokyo), we will carry out systematic investigations with chiral 3N forces within the shell model and their impact on nuclear structure and shell evolution. We have started to calculate the 3N force contributions to $T=0$ shell-model matrix elements, and as a first step will study ground-state energies and spectra from oxygen to silicon, where (except for the heavier proton-rich cases) the ground-state energies are known and the structure can also be accessed experimentally. We will analyze in detail the convergence properties with low-momentum NN and 3N interactions to second and third order in many-body perturbation theory for effective shell-model Hamiltonians.

Next, we will perform large-scale shell-model calculations for the full sd- and pf-shells, with specific attention to results and predictions that motivate experimental investigations within the CRC. In addition, we will include continuum contributions for loosely-bound nuclei through a Gamow-Hartree-Fock basis. We will advance the 3N forces frontier in the shell model to the chain of tin isotopes and study their pairing properties in comparison with energy-density-functional calculations based on low-momentum NN and 3N forces as pairing interaction.

We have started to carry out first calculations with two-body-current contributions in chiral EFT (which are determined fully at leading order by low-energy couplings in NN and 3N forces) for Gamow-Teller transitions and neutrinoless double-beta decay. Our preliminary first results show that two-body currents lead to important contributions for electroweak operators in medium-mass nuclei, especially for Gamow-Teller transitions. In medium-mass nuclei, the contributions from two-body currents are larger compared to light nuclei because the typical nucleon momenta are $\sim 100$ MeV. We will explore this exciting direction systematically up to the pf-shell and for the important cases of neutrinoless double-beta decay nuclear matrix elements.

**Coupled-cluster calculations of medium-mass nuclei with 3N forces**

With G. Hagen (ORNL), T. Papenbrock (ORNL/UT), S. Bacca (TRIUMF) and A. Nogga (FZ Jülich), we are presently carrying out the first Coupled-Cluster (CC) calculations for medium-mass nuclei. Our contribution is the calculation of NN and 3N interaction matrix elements in J-coupled scheme (and m-scheme for testing) and to explore the sensitivities to the input nuclear forces probed through cutoff dependence and variations of the $c_i$ couplings that
determine the long-range two-pion-exchange parts of the leading 3N forces. We have converged results for \(^4\)He and \(^{16}\)O at the CC singles and doubles (CCSD) level but are finding that triples corrections are larger with 3N forces included. Therefore, we will implement full triples (CCSDT) contributions at the normal-ordered two-body level. First milestone CC results with 3N forces will be for the closed-shell nuclei \(^4\)He (to compare with exact results), \(^{16}\)O and \(^{40}\)Ca, and for the helium-halo nuclei.

We will advance the 3N forces frontier to the chain of oxygen isotopes, \(^{15,16,17,21,22,23,24,25,27,28,29}\)O, and calcium isotopes, \(^{39,40,41,47,48,49,51,52,53,54,55,59,60,61,69,70,71}\)Ca, where these closed-subshell and particle attached/removed cases are accessible with the existing CC technology after the first milestone developments. We will use CC theory to benchmark the IM-SRG and many-body perturbation theory for valence-nucleon interactions used for the shell-model project area, and to develop and test tractable approximations to handle many-body interactions, for instance represented as density-dependent forces. We will advance CC theory with 3N forces to heavier nuclei, exploring calculations of the tin isotopes and the neutron-skin of lead.

**Systematics of ground and excited states with NN plus 3N interactions**

In addition to accurate ab-initio approaches, we will study the global systematics of different nuclear observables over a wide range of nuclei using approximation schemes starting from the same consistently transformed NN plus 3N Hamiltonians. We have developed a versatile toolbox of approximate methods to address ground-state properties and excitations throughout the whole nuclear chart. These methods include different forms of many-body perturbation theory (MBPT), such as low-order MBPT and Padé-, ladder- or ring-resummation techniques, on top of self-consistent Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) calculations.

We will extend the existing MBPT plus HF framework to include SRG-transformed NN plus 3N Hamiltonians. We have demonstrated the feasibility of such calculations using phenomenological 3N contact interactions already. Furthermore, we will extend the MBPT methodology to the treatment of excited states and the full set of ground-state observables including radii, density distributions and form factors. Besides the inclusion of the full 3N terms, we will investigate approximations for including the 3N contributions, e.g., in the form of a truncated normal-ordered Hamiltonian. We envision studying closed- and open-shell nuclei up to the Pb isotopic chain in this framework. In addition to ground-state properties we will address the systematics of excitation energies, in particular for the first \(^2^+\) excited states, in the framework of degenerate MBPT.

Again, the physics impact of these calculations is two-fold: They will provide critical information on the properties of the SRG-transformed chiral NN plus 3N interactions complementing the exact ab-initio calculations. We will be able to study the full range of nuclear masses, thus, providing constraints on the nuclear Hamiltonian. Deficiencies of the Hamiltonian, in particular regarding initial and induced multi-nucleon forces, will affect heavier nuclei much more severely. Already the reproduction of the experimental systematics of ground-state energies and charge radii is challenging.

In addition to constraining the Hamiltonian, we will be able to study a number of interesting nuclear structure questions. In addition to ground-state energies, radii and density distributions, we will continue to study pairing properties in a fully self-consistent HFB framework using NN plus 3N interactions. Beyond the ground states we will use MBPT for excited states in order to investigate the systematics of low-lying excitations in medium-mass and heavy nuclei. The whole complex of collective excitations, which is intimately related to the experimental program of the CRC, will be investigated in detail in project D2.
building on the input and on the results from this project.

**Advancing nuclear matter and studies of pairing in nuclei**

We have made significant progress in understanding nuclear and neutron matter based on chiral low-momentum NN and 3N interactions and their uncertainties. This opens the door to develop a universal nuclear energy density functional (UNEDF) based on nuclear forces and provides important constraints for nuclear astrophysics. A key next step is to include 3N and 4N interactions at N³LO, so that all nuclear force contributions to N³LO are taken into account. At least for neutron matter, our results show that these are the dominant uncertainties in the present calculations. The different parts of 3N and 4N forces at N³LO have been calculated in momentum space, so that the inclusion in nuclear and neutron matter calculations is considerably simpler than to develop the antisymmetrized JT-coupled 3N and 4N Jacobi matrix elements in a harmonic-oscillator basis needed for nuclei. The first nuclear and neutron matter calculations with N³LO 3N and 4N forces will include their contributions as density-dependent two-body interactions by summing the third and fourth particles over occupied states in the Fermi sea. In addition, the full 3N and 4N contributions will be evaluated at first and second order using Monte Carlo integration methods.

As a warm-up problem on nuclear forces and to balance the more technical project on N³LO 3N and 4N interactions, the junior researchers working in this area will first get to know nuclear forces by exploring their impact on pairing in nuclei. We will compare the pairing gaps in tin isotopes obtained from low-momentum NN and 3N interactions in energy-density-functional calculations to shell-model results based on the same interactions at first order and including polarization effects in the shell model.

**Merging Nuclear Structure and Reaction Theory**

Our advance with the IT-NCSM has opened a unique opportunity to merge ab-initio nuclear structure and reactions calculations. In collaboration with Petr Navrátil (TRIUMF) and Sofia Quaglioni (LLNL) we have combined the IT-NCSM for the description of low-lying states of the target nucleus with the Resonating Group Method (RGM) for the description of the relative motion of projectile nucleon and target nucleus. As compared to the original NCSM/RGM the use of the importance truncation allows us to access heavier
nuclei and larger model spaces, which is important for the convergence of the RGM kernels. This scheme provides a consistent ab-initio approach to low-energy reactions using the same realistic Hamiltonian at all stages of the calculation.

This framework gives direct access to low-energy reaction observables relevant for nuclear astrophysics, spanning a bridge to project D3. An example is the astrophysical S-factor for the proton-capture reaction $^7\text{Be}(p,\gamma)^8\text{B}$, which has considerable impact on the solar model and is crucial for understanding the solar neutrino flux. In addition to these applications, several methodological developments are planned, e.g., the extension to heavier projectiles and the inclusion of full or approximate 3N interactions at the RGM level.