# Ab Initio Nuclear Structure Theory with Chiral NN+3N Interactions

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Low-energy nuclear theory has entered an era of ab initio nuclear structure and reaction calculations based on QCD. One of the most promising paths from QCD to nuclear observables employs Hamiltonians constructed within chiral effective field theory as starting point for precise ab initio studies. However, the full inclusion of chiral two- plus three-nucleon (NN+3N) interactions in exact and approximate many-body calculations poses a formidable challenge. We discuss recent breakthroughs that allow for ab initio calculations for ground states and spectra of nuclei throughout the p- and the lower sd-shell with full 3N interactions using consistent Similarity Renormalization Group (SRG) transformations and the Importance Truncated No-Core Shell Model (IT-NCSM). Moreover, we discuss extensions of these ab initio calculations to heavy nuclei within coupled cluster theory using a normal ordering approximation of the 3N interaction.

## §1. Introduction

One of the most exciting frontiers in ab initio nuclear structure and reaction theory today is the full exploitation of low-energy QCD, e.g., through chiral effective field theory (EFT), for the prediction of a variety of experimentally relevant observables in a wide range of nuclear masses. Eventually, the aim is to establish a unified approach to nuclear structure and reaction physics that is solidly rooted in low-energy QCD. By starting from the symmetries and relevant degrees of freedom of low-energy QCD and using a sequence of exact or well-controlled and improvable theoretical and computational steps to arrive at nuclear structure observables, we will enable rigorous predictions that, after confrontation with experiment, allow for a validation of the underlying theoretical concepts.

One of the most universal implementations of this general scheme employs three stepping stones to bridge the gap from low-energy QCD to nuclear structure and reaction observables: The starting point are consistent nuclear interactions derived within chiral EFT. At present, high-precision chiral two-nucleon (NN) interactions are available at order $\mathrm{N^3LO}$[1),2)] and chiral three-nucleon (3N) at order $\mathrm{N^2LO}$.[3),4)] Developments are under way to include the chiral 3N interaction consistently at order $\mathrm{N^3LO}$.[5),6)]

In a next step, based on the NN+3N Hamiltonian obtained from chiral EFT, we use a unitary transformation to pre-diagonalize the Hamiltonian. From a practical point of view this pre-diagonalization aims to improve the convergence behavior of the subsequent many-body calculation and thus facilitate converged calculations in systems that are not accessible with the initial Hamiltonians. From a physics point of view, the pre-diagonalization tames parts of the interaction that induce strong cor-

relations in the many-body states. However, since the transformation is unitary, this simplification of the many-body states results in a complication of the transformed operators, such that observables are invariant. We focus on unitary transformations that are independent of the specific many-body method and model space used later-on. Thus we obtain a universal transformed Hamiltonian and accompanying transformed observables that can be used in different many-body methods. In the following we focus on the Similarity Renormalization Group as a simple and flexible tool to perform this unitary transformation.[7),8)]

In a final step we solve the many-body problem for the transformed Hamiltonian using a variety of many-body methods tailored for the mass range and the observables of interest. For the p-shell and the lower sd-shell the No-Core Shell Model and its extension, the Importance Truncated No-Core Shell Model, are the methods of choice. These ab initio methods give access to ground states and low-lying excitations and all corresponding observables based on the full NN+3N Hamiltonian without approximation. However, the inclusion of the 3N interaction is a computational challenge. By combining a new technology for handling 3N matrix elements with the importance truncation we recently pushed the limit for ab initio calculations with full chiral 3N interactions to much heavier nuclei and larger model spaces.

To access even heavier systems, beyond the mid sd-shell, with 3N interactions we have to resort to a different many-body method. If we focus on ground states of closed-shell nuclei the coupled cluster approach is the method of choice regarding accuracy and efficiency. As an alternative to the full inclusion of 3N interactions, as it is done in the IT-NCSM, one can consider the 3N contributions in a normal-ordering approximation which dramatically reduces the computational effort. In this framework, coupled-cluster theory with a normal-ordered 3N interactions truncated at the two-body level, the whole nuclear chart can be covered.

## §2. Similarity Renormalization Group with 3N Interactions

The Similarity Renormalization Group (SRG) is one of the simplest methods to pre-diagonalize a Hamiltonian through a unitary transformation and, at the same time, to transform all other relevant operators consistently. Its simplicity results from the fact that the transformation is formulated in terms of a first-order differential equation in a flow-parameter $\alpha$, the so-called flow equation,

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \quad \text{with} \quad \eta_\alpha = (2\mu)^2 [T_{\mathrm{int}}, H_\alpha] \,, \tag{2·1}$$

where $\eta_\alpha$ is the dynamical generator of the transformation. In the following we will restrict ourselves to the above definition of the generator as a commutator of the intrinsic kinetic energy and the evolving Hamiltonian, but other choices are possible and are under investigation. Analogous evolution equations can be formulated for any observable $O_\alpha$, such as electromagnetic multipole operators, radii, and densities.

To solve the flow equation numerically we use a $n$-body basis representation, thus the Fock-space operator equation (2·1) is converted into a set of coupled ordinary differential equations for the $n$-body matrix elements of the operator $H_\alpha$. This entails

a truncation of the evolved operator to contributions up to $n$-body operators. At present we are able to handle the evolution up to the $n = 3$ level, which allows us to include all two- and three-body terms of the evolved Hamiltonians, but not the four-body terms that might be induced by the unitary transformation. In the following we study three different truncations of the SRG-evolved Hamiltonian: *(i) NN-only*: we start with an initial NN interaction and keep the two-body terms only; *(ii) NN+3N-induced*: we start with an initial NN interaction and keep two- and induced three-body terms; *(iii) NN+3N-full*: we start with an initial NN+3N interaction and keep the two- and all three-body terms.

The omission of induced many-body terms results in a formal violation of unitarity of the transformation in $A$-body space. If the omitted many-body terms are relevant, one will observe a dependence of the eigenvalues of the Hamiltonian on the transformation due to the loss of unitarity. We can use a variation of the flow-parameter $\alpha$ as a diagnostic tool to probe the contribution of omitted many-body terms. Any dependence on $\alpha$ of, e.g., the ground-state energy, in an exact many-body calculation signals the importance of omitted induced many-body terms.

## §3. Importance Truncated No-Core Shell Model

In a first application of the SRG-transformed chiral NN+3N interactions in nuclear structure calculations beyond the lightest isotopes, we employ the Importance Truncated No-Core Shell Model (IT-NCSM) developed in our group.[9),10)] It makes use of the fact that many of the NCSM basis states are irrelevant for the description of a set of low-lying states. Guided by many-body perturbation theory, one can define a measure for the importance of individual basis states and discard states with an importance measure below a threshold value, thus reducing the dimension of the matrix eigenvalue problem. Through a sequence of IT calculations for different thresholds and an a posteriori extrapolation of all observables to vanishing threshold, we can recover the full NCSM results up to extrapolation errors.[10)] The IT-NCSM together with a novel storage and management scheme for the 3N matrix elements allows us to perform ab initio calculations including 3N interactions without any approximation for nuclei in the upper p- and lower sd-shell. All observables that are accessible in the NCSM, such as ground-state and excitation energies, electromagnetic moments and transitions, radii and densities, etc., are accessible in the IT-NCSM as well.

Using the IT-NCSM we can study the three different truncations of the SRG-evolved chiral Hamiltonian and, thus, the role of initial chiral 3N interactions and of SRG-induced 4N (and many-body) terms. In Figure 1 we summarize IT-NCSM results for the ground-state energies of $^{12}$C and $^{16}$O as function of model-space size $N_{\max}$ and flow parameter $\alpha$. First of all, we note that we are able to reach unprecedented model-space sizes of $N_{\max} = 12$ in these upper p-shell nuclei including full 3N interactions. This is sufficient to converge the ground-state energies for the softer interactions. For the NN-only Hamiltonian, for which all 3N-terms are discarded, we observe a strong $\alpha$-dependence of the converged energies hinting at important induced 3N terms that have been omitted. Their inclusion at the NN+3N-induced

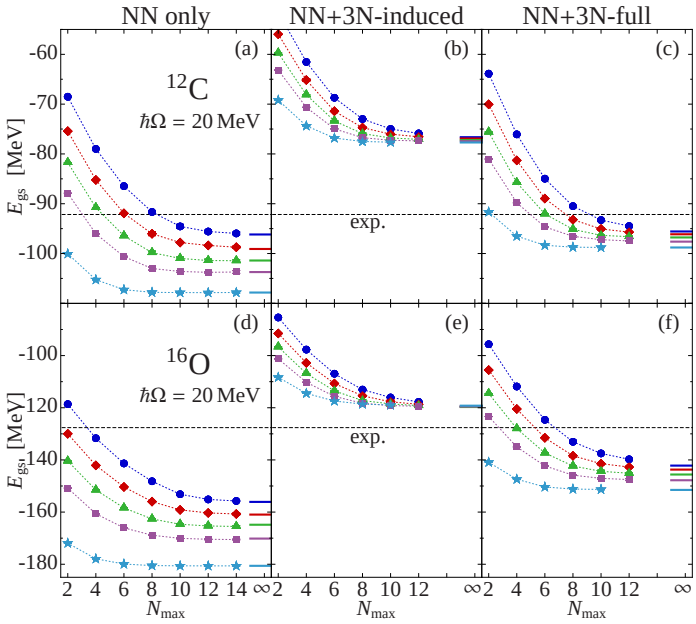


Fig. 1. IT-NCSM ground-state energies for $^{12}$C and $^{16}$O as function of $N_{\max}$ for the three types of Hamiltonians (see column headings) for a range of flow parameters: $\alpha = 0.04\,\mathrm{fm}^4$ (●), $0.05\,\mathrm{fm}^4$ (♦), $0.0625\,\mathrm{fm}^4$ (▲), $0.08\,\mathrm{fm}^4$ (■), and $0.16\,\mathrm{fm}^4$ (★). Taken from Ref.[11)]

level eliminates the $\alpha$-dependence and leads to a sizable shift of the ground-state energies. This means that induced 4N terms originating from the initial NN interaction are irrelevant and that the energies obtained with the NN+3N-induced Hamiltonian correspond to the exact ground-state solution of the initial NN Hamiltonian. If we now include the initial 3N interaction, i.e., if we use the NN+3N-full Hamiltonian, we observe a re-emergence of the $\alpha$-dependence. Thus the inclusion of initial 3N interaction generates induced 4N terms that are omitted. These 4N terms are irrelevant for nuclei in the lower p-shell, but their effect increases rapidly with increasing mass number.[11),12)]

Not all observables are affected by those induced 4N terms. If we consider excitation energies, i.e. energy differences instead of absolute energies, the $\alpha$-dependence is very small once convergence is reached. An example is shown in Figure 2, where the excitation spectrum of $^{12}$C obtained for the three different truncations of the Hamiltonian is depicted for two different values of $\alpha$. The spectra for the two flow parameters are practically on top of each other proving that quantitative calculations of excitation spectra are possible even without including the induced 4N terms. Crucial tests of the predictive power of chiral NN+3N interaction for spectra and spectroscopy of nuclei in the upper p- and lower sd-shell are thus possible.

## §4. Coupled Cluster Theory

To extend these studies to even heavier systems, we can use the SRG-evolved chiral NN+3N Hamiltonians in the context of Coupled Cluster Theory. At the simplest

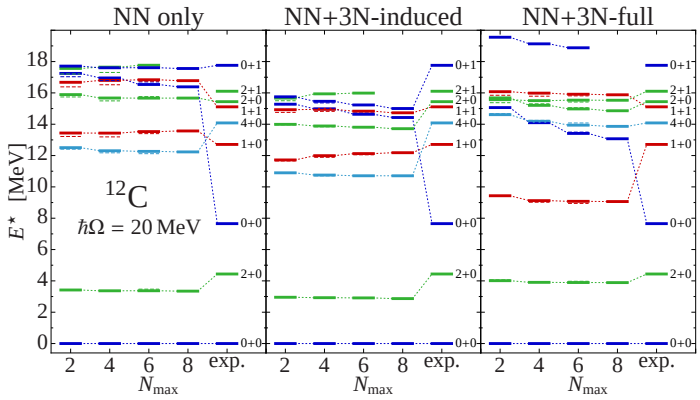


Fig. 2. Excitation spectrum for the lowest positive-parity states (labelled $J\pi T$) in $^{12}$C for the NN-only, the NN+3N-induced, and the NN+3N-full Hamiltonian with $\alpha = 0.08\,\mathrm{fm}^4$. The thin dashed bars (mostly hidden) show results for $\alpha = 0.0625\,\mathrm{fm}^4$. Take from Ref.[11)]

level, the Coupled Cluster with Singles and Doubles (CCSD) approximation,[13)] we already obtain a very good approximation for the ground-state energy of closed-shell nuclei, which can be improved by including triples corrections. The 3N interactions can be included either exactly or in the so-called Normal-Ordered Two-Body (NO2B) approximation. We have performed detailed benchmarks of this approximation and found it to be accurate to about 1% for ground-state energies.[12)] The use of the NO2B approximation reduces the computational cost dramatically, since technically only two-body terms have to be included into the many-body calculation. In combination CCSD and NO2B are able to predict ground-states of closed-shell nuclei throughout the whole nuclear chart using chiral NN+3N interactions as input.

As an example, Figure 3 shows results of the first CCSD calculations for Calcium isotopes including SRG-evolved chiral NN+3N Hamiltonians. In addition to a confirmation of the emergence of induced 4N terms in heavier systems, we demonstrate that by lowering the cutoff of the initial chiral 3N interaction within a sensible range given by chiral EFT the induced 4N contributions are substantially reduced. This paves the way to accurate ab initio calculations using chiral NN+3N interaction up to the heaviest nuclei.

## §5. Conclusions

We have developed the formal and computational tools to enable ab initio calculations of nuclear structure based on chiral NN+3N interactions for a wide range of masses and observables. The developments open a vast domain of applications, e.g., for the description of the spectroscopy of p- and sd-shell nuclei and for accurate ab initio mass calculations along isotopic chains up to the driplines. We are also in the process of implementing the 3N technology into calculations for scattering and reactions of light nuclei in the NCSM combined with the Resonating Group Method. Together this opens completely new territory for ab initio nuclear structure and reaction theory, which we will explore in the future.

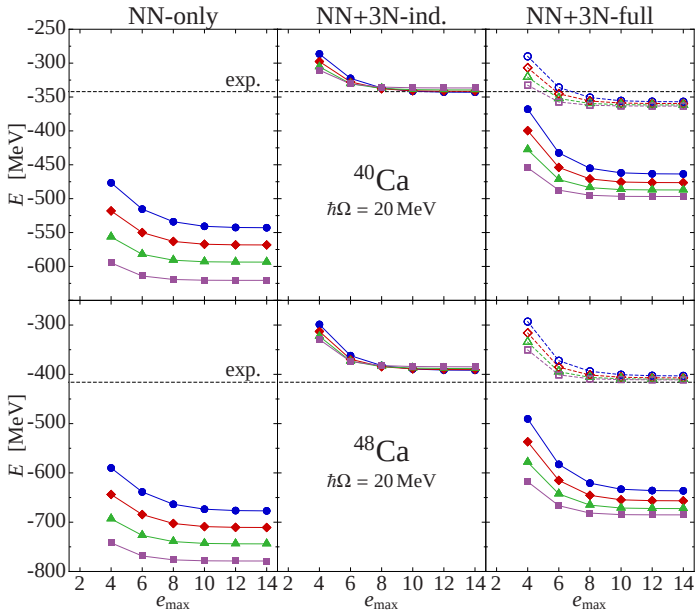


Fig. 3. CCSD ground-state energies for $^{40}$Ca and $^{48}$Ca for the three types of Hamiltonians using the NO2B approximation for a range of flow parameters: $\alpha = 0.04\,\mathrm{fm}^4$ (●), $0.05\,\mathrm{fm}^4$ (♦), $0.0625\,\mathrm{fm}^4$ (▲), and $0.08\,\mathrm{fm}^4$ (■). The filled symbols for the NN+3N-full Hamiltonian are for the standard chiral 3N interaction with cutoff 500 MeV, the open symbols for a modified 3N interaction with cutoff 400 MeV. Taken from Ref.[12)]

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