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Ab Initio Nuclear Structure Theory: From Few to Many

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Abstract We summarize recent advances in ab initio nuclear structure theory, aiming to connect few- and many-body systems in a coherent theoretical framework. Starting from chiral effective field theory to construct the nuclear Hamiltonian and the similarity renormalization group to soften it, we address several many-body approaches that have seen major developments over the past few years. We show that the domain of ab initio nuclear structure theory has been pushed well beyond the p-shell and that quantitative predictions connected to QCD via chiral effective field theory are becoming possible all the way from the proton to the neutron drip line up into the medium-mass regime.

Keywords ab initio nuclear structure theory · chiral effective field theory · from no-core shell model to coupled-cluster theory

1 Introduction

Low-energy nuclear structure and reaction theory underwent a paradigm shift over the past few years. Ab initio nuclear theory is evolving into a systematic theory of nuclear properties for stable and exotic nuclei that is rooted in QCD. This evolution is driven by simultaneous advances in different areas: (i) the understanding of QCD in the low-energy regime through chiral effective field theory (EFT); (ii) innovations in many-body theory giving access to new regions of the nuclear chart and new observables; (iii) new algorithms and increased computational resources that help to tackle exceedingly complex problems numerically; (iv) exciting present and future opportunities for experiments on nuclei far-off stability. The recent success of ab initio nuclear theory emerges from the interplay of these areas and a coherent effort of the different sub-communities is exceedingly important.

In this contribution we touch upon a few recent advances within ab initio many-body theory, which aim towards providing a universal theoretical framework connected to QCD via chiral EFT with controlled and quantified uncertainties.

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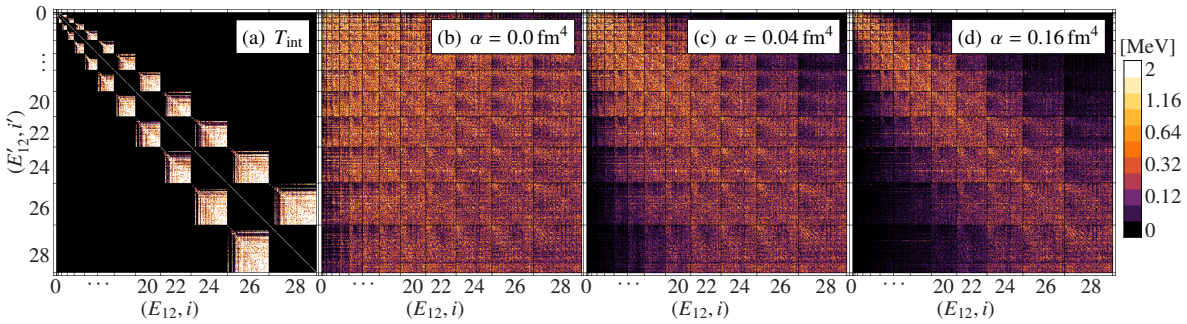

Fig. 1 Effect of the SRG evolution on the matrix elements of the NN+3N-full interaction in a three-body harmonic-oscillator Jacobi basis. Panel (a) shows the kinetic energy, panels (b) to (d) the interaction part of the evolving Hamiltonian. Light colors represent large absolute values and dark colors represent matrix elements near zero. Taken from Ref. [26].

2 Nuclear Hamiltonian

2.1 Interactions from Chiral EFT

Chiral effective field theory has become the most widely used approach to construct nuclear interaction capturing the low-energy dynamics and relevant degrees of freedom of QCD [18; 11]. In many ab initio nuclear structure methods, the nucleon-nucleon (NN) interactions derived from chiral EFT have replaced many of the traditional realistic interactions. There are a number of conceptual and practical reasons for the success of chiral EFT interactions, e.g., the possibility to derive consistent two-nucleon, three-nucleon (3N) and multi-nucleon interactions as well as electromagnetic and weak current operators, and the possibility to systematically improve the description by including higher orders of the chiral expansion.

So far, the chiral EFT Hamiltonian that has most widely been used consists of a high-precision NN interaction at next-to-next-to-next-to-leading order (N^3LO) by Entem and Machleidt [8] along with a 3N interaction at next-to-next-to-leading order (N^2LO) in a local formulation by Navrátil [19] with low-energy constants c_D and c_E fit to the $A = 3$ binding energies and the triton half-life [12]. Obviously, this Hamiltonian does not include NN and 3N interactions at consistent order. The missing 3N contributions at N^3LO have been derived recently [1; 2] and a collaborative effort is under way to compute the numerical matrix elements suitable for inclusion in standard many-body approaches (LENPIC collaboration). Apart from the consistent Hamiltonian at N^3LO several consistent Hamiltonians at N^2LO are available already, e.g., the Hamiltonians by Epelbaum et al. [10; 9] or the recent N^2LO-optimized Hamiltonians [7].

2.2 Similarity Renormalization Group

Although the chiral interactions are softer than traditional realistic interactions, their direct inclusion into a configuration-space many-body calculation requires huge model spaces in order to obtain convergence. An efficient tool to accelerate the convergence of the subsequent many-body calculation are unitary transformations. The so-called similarity renormalization group (SRG) [23; 6] has become one of the most popular of these transformations, mainly because of its simplicity and flexibility.

The SRG is a continuous unitary transformation formulated in the language of renormalization group flow-equations and governed by a flow parameter α, which can be used to drive the Hamiltonian towards band-diagonal form with respect to a specific many-body basis, depending on the generator. The transformed Hamiltonian H_α and any other consistently transformed observable O_α are determined by Heisenberg-like first-order differential equations

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} H_\alpha = [\eta_\alpha, H_\alpha]\,, \qquad \frac{\mathrm{d}}{\mathrm{d}\alpha} O_\alpha = [\eta_\alpha, O_\alpha]\,, \qquad \eta_\alpha = (2\mu)^2 [T_{\rm int}, H_\alpha], \tag{1}$$

with η_α being the dynamic generator of the transformation. The flexibility of the SRG results from the fact that any antihermitian operator can be used as generator. In the following we restrict ourselves to the definition of the generator as commutator of the intrinsic kinetic energy $T_{\rm int}$ with the transformed Hamiltonian, which

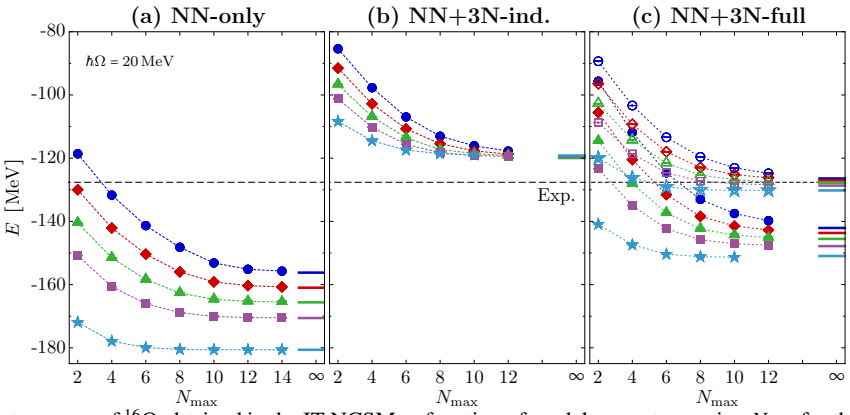

Fig. 2 Ground-state energy of ^{16}O obtained in the IT-NCSM as function of model-space truncation $N_{\max}$ for the NN-only (a), the NN+3N-induced (b), and the NN+3N-full Hamiltonian (c). The different symbols correspond to different SRG flow parameters: $\alpha = 0.04\,\mathrm{fm}^4$ (●), $0.05\,\mathrm{fm}^4$ (◆), $0.0625\,\mathrm{fm}^4$ (▲), $0.08\,\mathrm{fm}^4$ (■), $0.16\,\mathrm{fm}^4$ (★). The filled symbols in panel (c) show results with the chiral 3N interaction for $\Lambda_{3\mathrm{N}} = 500\,\mathrm{MeV}/c$, open symbols for $\Lambda_{3\mathrm{N}} = 400\,\mathrm{MeV}/c$.

is common in context of nuclear physics (see, e.g., Ref. [5]). However, other choices of the generator are possible and under investigation.

In order to solve the flow equations numerically, we convert Eq. (1) into matrix-element representation with respect to an n-body basis. The effect of the SRG transformation on the matrix elements of the NN+3N interaction in the three-body harmonic-oscillator Jacobi basis is illustrated in Fig. 1. The left-hand panel shows the initial interaction, i.e., $\alpha = 0\,\mathrm{fm}^4$, exhibiting large matrix elements even far off the diagonal. The middle and right-hand panels show the SRG-transformed matrix elements for flow parameters $\alpha = 0.04\,\mathrm{fm}^4$ and $0.16\,\mathrm{fm}^4$, respectively. Evidently, the SRG transformation causes a prediagonalization of the matrix, i.e., a decoupling of the high- and low-energy states and thus an improvement of the convergence of the many-body calculation.

The projection of the operator equations (1) onto an n-body Hilbert space eliminates flow-induced operator contributions beyond the n-body level. Thus, when solving the flow equation in a three-body matrix representation, e.g., we will discard induced four- and multi-nucleon contributions. The lack of these contributions destroys the formal unitarity of the SRG transformation and can induce a dependence of the converged energy eigenvalues on the flow parameter α. Therefore, the flow parameter provides a valuable tool to measure the impact of omitted induced many-body contributions.

We routinely perform the SRG evolution in three-body space, i.e., we include initial and SRG-induced 3N interactions. To study the anatomy of the SRG-evolved Hamiltonians, we use three different truncations: *(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. First studies of SRG evolutions in four-body space are in progress and will give access to initial and induced 4N interactions in the future.

3 Nuclear Many-Body Problem — Ab Initio

3.1 No-Core Shell Model

Traditionally, the lower p-shell was the domain of ab initio nuclear structure calculations over the past decade, with the Green's function Monte Carlo (GFMC) approach and the no-core shell model (NCSM) being the most prominent representatives. A series of developments and improvements, both, conceptually and computationally have created opportunities for NCSM-type ab initio calculations extending up into the lower sd-shell. Among those developments is the importance truncation (IT) of the NCSM model space [22; 21; 26]. The IT-NCSM together with a novel treatment of the 3N matrix elements, based on storing JT-coupled matrix elements and their efficient on-the-fly decoupling, enables ab initio calculations including explicit 3N interactions in huge model spaces in particular for nuclei in the upper p- and lower sd-shell [26].

The first ab initio calculations with SRG-evolved chiral NN+3N interactions in the upper p-shell [24; 26] have demonstrated that sizable SRG-induced 3N contributions emerge from the initial chiral NN interaction.

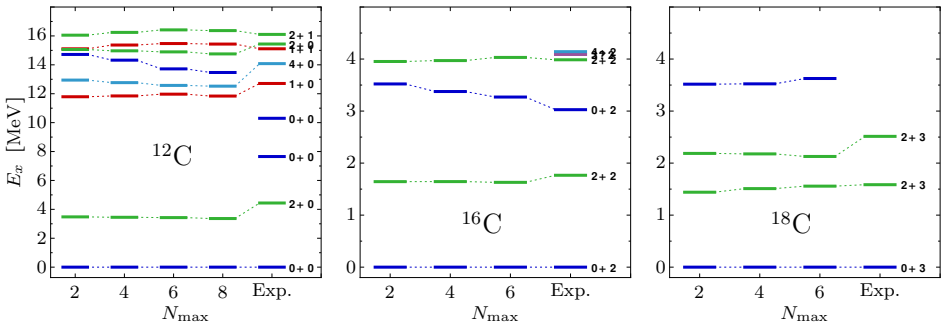

Fig. 3 Excitation spectrum of ^{12}C, ^{16}C, and ^{18}C obtained in the IT-NCSM for $\hbar\Omega = 16\,\mathrm{MeV}$, $\alpha = 0.08\,\mathrm{fm}^4$ with the NN+3N-full Hamiltonian for reduced 3N cutoff $\Lambda_{3\mathrm{N}} = 400\,\mathrm{MeV}/c$.

This is illustrated in Fig. 2(a) and (b), where the ground-state energy of ^{16}O obtained in the IT-NCSM with the NN-only and the NN+3N-induced Hamiltonian is depicted as function of the model-space parameter $N_{\max}$. When including the initial chiral 3N interaction, SRG-induced 4N contributions become relevant and reveal themselves through the flow-parameter dependence of the results with the NN+3N-full Hamiltonian as shown in Fig. 2(c). We note that the overbinding visible in Fig. 2(c) for the NN+3N-full Hamiltonian could result entirely from the omission of the induced 4N interactions, which are known to be repulsive, and does not necessarily imply a problem with the initial chiral Hamiltonian.

One way to reduce the contribution of SRG-induced 4N interactions is to reduce the cutoff $\Lambda_{3\mathrm{N}}$ of the initial chiral 3N interaction. Already a reduction from the common value of $\Lambda_{3\mathrm{N}} = 500\,\mathrm{MeV}/c$ to $\Lambda_{3\mathrm{N}} = 400\,\mathrm{MeV}/c$ reduces the size of the induced 4N contributions significantly. For the latter 3N interaction we have readjusted the c_E parameter to reproduce the ^{4}He ground-state energy obtained with the bare interaction and kept all other low-energy constants as in Ref. [12]. The reduction of the flow-parameter dependence and thus the suppression of the induced 4N interactions is clearly visible in Fig. 2(c). For $\Lambda_{3\mathrm{N}} = 400\,\mathrm{MeV}/c$ the SRG-evolved Hamiltonian at the NN+3N-full level is to a good approximation unitarily equivalent to the initial chiral NN+3N Hamiltonian.

One of the typical applications of the NCSM is the description of the spectroscopy of light nuclei. Within the IT-NCSM we can extend these studies to the upper p- and lower sd-shell with explicit inclusion of chiral 3N interactions. As an example we present the excitation spectra of selected carbon isotopes in Fig. 2 obtained with the chiral NN+3N Hamiltonian for $\Lambda_{3\mathrm{N}} = 400\,\mathrm{MeV}/c$. We stress that since the Hamiltonian was determined using experimental data up to $A \leq 4$, these calculations are completely parameter-free. We find a remarkable agreement of the spectra obtained in the IT-NCSM with experimental data, even when approaching the drip line. This is clear evidence for the predictive power of chiral NN+3N Hamiltonians beyond the lightest isotopes. As this example shows, advances in chiral EFT for NN and 3N interactions together with innovative methods in many-body theory plus computational resources and algorithmic developments enable ab initio calculations of nuclei and observables that are just becoming accessible in experiment.

3.2 Coupled Cluster, In-Medium SRG & Co.

The regime of medium-mass nuclei is a particularly exciting field for new developments in many-body theory. Within the past few years several new many-body methods have been introduced that are inspired by approaches in atomic and molecular physics, quantum chemistry, or condensed matter physics, among those are advanced versions of coupled-cluster theory [13], self-consistent Green's function approaches [27], and the so-called in-medium similarity renormalization group (IM-SRG) [28]. All of these methods are capable of describing medium-mass and even heavy nuclei with closed sub-shells using NN interactions. Various extensions to near closed-shell and to true open-shell nuclei are being explored in all approaches.

The inclusion of explicit 3N interactions poses a significant formal and computational challenge for all methods. Recently, we have performed the first large-scale coupled-cluster calculations for ground states of closed-shell medium-mass nuclei including explicit 3N interactions up to the level of triples corrections [3; 4]. In this framework we have benchmarked approximate schemes for the inclusion of the 3N interaction. The most natural and powerful approximation scheme is based on the normal-ordered 3N interaction with respect to the coupled-cluster reference state. Truncating the normal-ordered 3N operator at the two-body level results

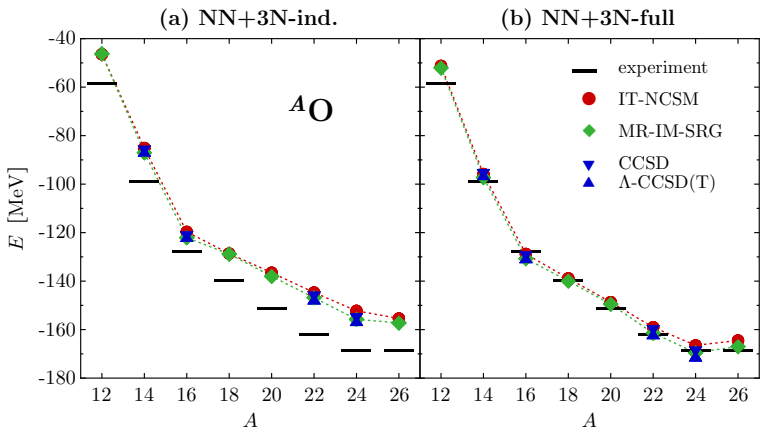

Fig. 4 Ground-state energies for the even oxygen isotopes obtained with the IT-NCSM (●), the multi-reference in-medium SRG (◆), and the coupled-cluster method with singles and doubles (▼) and with the Λ-CCSD(T) triples corrections (▲). Panel (a) shows results for the NN+3N-induced Hamiltonian at $\alpha = 0.08\,\mathrm{fm}^4$, panel (b) with the NN+3N-full Hamiltonian with $\Lambda_{3N} = 400\,\mathrm{MeV}/c$ and $\alpha = 0.08\,\mathrm{fm}^4$. Adapted from [15].

in an enormous simplification of the many-body calculations, since technically only two-body terms appear. Nonetheless, this approximation provides quite accurate results. From the direct comparison of the CC results with explicit 3N interactions to the ones using the normal-ordered two-body approximation we can conclude that both calculations agree to better than 1% while the computational cost is reduced dramatically [25; 3].

Normal-ordering in its single-reference or more advanced multi-reference formulations is also at the heart of the in-medium SRG. It combines a SRG evolution in many-body space, which decouples particle-hole excitations from the reference state, with the normal-ordering approximation to absorb induced many-body terms. In contrast to the free-space SRG, discussed in Sec. 2.2, which is used to pre-condition the Hamiltonians for subsequent many-body calculations, the in-medium SRG directly serves as a many-body calculation for the nuclear ground state [16]. The expectation value of the evolved Hamiltonian with the reference state, which is just the normal-ordered zero-body contribution of the reference state, yields the ground-state energy of the system.

We demonstrated the power and accuracy of the in-medium SRG for open and closed-shell oxygen isotopes very recently [15]. Using the Hamiltonians discussed above, we computed the ground-state energy of the even oxygen isotopes from proton to neutron drip line in the IT-NCSM, the in-medium SRG, and for the closed sub-shells in coupled-cluster theory up to the doubles level without and with triples corrections. The results are summarized in Fig. 4. The ab initio IT-NCSM calculations are computationally very demanding. Nevertheless, we were able to perform calculations up to $N_{\max} = 12$ even for ^{26}O, which is clearly beyond the reach of the conventional NCSM. The IT-NCSM results serve as a reference point for the in-medium SRG and coupled-cluster calculations, which both use the normal-ordered two-body approximation to include the NN+3N Hamiltonians and different truncations in the many-body expansion.

The agreement among the different methods shown in Fig. 4 is remarkable – within the expected uncertainties, the results agree with each other. This proves that the many-body problem is well under control and that calculations with quantified uncertainties are now possible, even in this mass region. A second remarkable point is the agreement of the results for the NN+3N-full Hamiltonian with the experimental ground-state energies. Again we stress that these are parameter-free calculations using a Hamiltonian that was completely determined in $A \leq 4$ systems. This demostrates that the chiral Hamiltonians contain the physics relevant for a quantitative ab initio description of nuclei at extreme isospins. As has been pointed out in valence-space shell model calculations [20] and coupled-cluster calculations with phenomenological 3N effects [14], the 3N interaction is necessary to reproduce the drip line at ^{24}O.

The corresponding calculations with in-medium SRG and coupled-cluster theory for isotopic chains of heavier elements, in particular the calcium and nickel isotopic chains, will be available soon. Work towards the description of excited states and spectroscopic observables is under way and promises to provide a complete ab initio picture of nuclear structure also in the medium-mass regime.

4 Conclusion & Outlook

Ab initio nuclear structure theory has developed rapidly over the past years, expanding its reach from few- to many-nucleon systems. It has ventured into new regions of the nuclear chart and strengthened its foundations in low-energy QCD. There is an unprecedented diversity of innovations aiming to advance ab initio theory and to connect it to the exciting probes into nuclear structure and reaction phenomena that present and future experiments offer.

The coming years will see further important advances, some of them in-line with the philosophy of the few-body community. We will work towards the consistent inclusion of the inputs from chiral EFT into nuclear structure physics, this includes consistent chiral Hamiltonians at N^3LO and the corresponding electro-weak current operators at the two-body level with consistent SRG transformation. We have started already to rigorously quantify the uncertainties of the various many-body frameworks, a next step will be the systematic propagation of the errors from the chiral EFT inputs (due to truncations and uncertainties in the low-energy constants) to nuclear structure observables. The ab initio description of continuum effects and reaction processes is advancing very quickly. Recently, we presented first scattering calculations in the resonating group method combined with the NCSM with NN+3N interactions at the same level of sophistication as in the structure calculation [17]. Finally, the tools developed in ab initio nuclear structure can be generalized to include additional constituents. In particular the inclusion of hyperons, leading to ab initio hypernuclear structure theory, opens new fields of application. The future of ab initio nuclear theory is bright and exciting!

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