From Chiral EFT Interactions to Ab Initio Nuclear Structure

Robert Roth[*]**, Joachim Langhammer, Angelo Calci and Sven Binder**
Institut für Kernphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany
E-mail: robert.roth@physik.tu-darmstadt.de

Chiral effective field theory provides nuclear interactions rooted in Quantum Chromodynamics in a systematic and consistent manner. To assess the quality and predictive power of chiral two-nucleon (NN) and three-nucleon (3N) interactions, ab initio calculations of a variety of nuclear observables are crucial. However, the inclusion of chiral 3N interactions into exact many-body calculations is demanding and computationally expensive. Recently, we completed a number of key developments which permit ab initio calculations of ground and low-lying excited states of p- and sd-shell nuclei with full 3N interactions in the Importance-Truncated No-Core Shell Model using consistent Similarity Renormalization Group transformations of the NN+3N Hamiltonian. The explicit treatment of 3N interactions without approximations allows for first studies of the dependence of nuclear-structure observables on the details of chiral interactions. We present first results of sensitivity studies with respect to variations of the low-energy constants and the chiral cutoff of the chiral 3N interactions. Our results hint at missing operator structures in the leading chiral 3N interactions which seem to be necessary to describe certain excited states in p-shell nuclei properly.

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[*]Speaker.

1. Introduction

Today, chiral effective field theory (chiral EFT) provides the most systematic approach to nuclear structure calculations using Hamiltonians based on Quantum Chromodynamics (QCD). Starting from nucleons and pions as relevant degrees of freedom and the symmetries of low-energy QCD, chiral EFT provides nuclear two-, three- and multi-nucleon interactions as well as current operators in a consistent way. A remaining challenge is to incorporate these QCD-based Hamiltonians in ab-initio nuclear structure and reaction calculations, in order to make precise predictions or to validate and constrain the chiral EFT description of nuclear forces by comparison to experiment.

The most advanced nuclear Hamiltonian from chiral EFT available in terms of matrix elements at the moment consists of a high-precision two-nulceon (NN) interaction at N^3LO [1, 2] along with a chiral three-nucleon (3N) force at N^2LO [3, 4]. Computations are underway to provide matrix elements of the 3N force consistently at order N^3LO [5, 6].

Obviously, the direct inclusion of these Hamiltonians into nuclear structure calculations is desirable. However, this requires huge and often intractable model spaces to account for the strong short-range correlations generated by the bare interactions. One way to tame these correlations is to soften the Hamiltonian by means of a unitary transformation, for example in the framework of the Similarity Renormalization Group (SRG) [7, 8]. The resulting transformed Hamiltonians exhibit an improved convergence behavior and, thus, facilitate the subsequent many-body calculations. When starting from chiral NN+3N Hamiltonians the SRG transformation can be and has to be carried out consistently, i.e., the NN and 3N interactions have to be evolved simultaneously. Since the SRG-transformation does not dependent on the nucleus or the many-body model-model space, we arrive at a universal transformed Hamiltonian with favorable convergence behavior that can be employed in a variety of many-body methods.

In this proceedings article we present nuclear structure calculations employing SRG-evolved NN+3N Hamiltonians from chiral EFT in the No-Core Shell Model (NCSM) [9, 10] and its extension, the Importance-Truncated No-Core Shell Model (IT-NCSM) [11, 12]. These ab initio methods are applicable for nuclei up to the lower *sd*-shell and yield ground states as well as low-lying excited states including all relevant observables. Since the inclusion of 3N forces is computationally demanding, we have developed new approaches for handling the 3N matrix elements. Together with the importance truncation, these techniques permit ab initio calculations for larger particle numbers and larger model spaces than before. We emphasize that all 3N interaction terms are included explicitly and without any approximation. Furthermore, the uncertainties of the many-body approach are controlled and quantified—this uncertainty quantification is a defining element of modern ab initio approaches. Eventually, this allows for a rigorous study of the sensitivity of nuclear structure observables on the chiral EFT input for the Hamiltonian, e.g., the low-energy constants (LECs) or cutoffs. We present first steps towards these sensitivity studies in this article.

For nuclei beyond the *sd* shell one would resort to other many-body methods. These are beyond the scope of this discussion, however, we note that we have made significant progress in including the explicit 3N interaction in the medium-mass regime using the Coupled Cluster (CC) approach [13]. This allows for rigorous benchmarks of approximate treatments of the 3N interaction, which we completed for the so called Normal-Ordered Two-Body (NO2B) approximation of the 3N interaction [14, 13, 15]. We found this approximation to be quite accurate, while it reduces
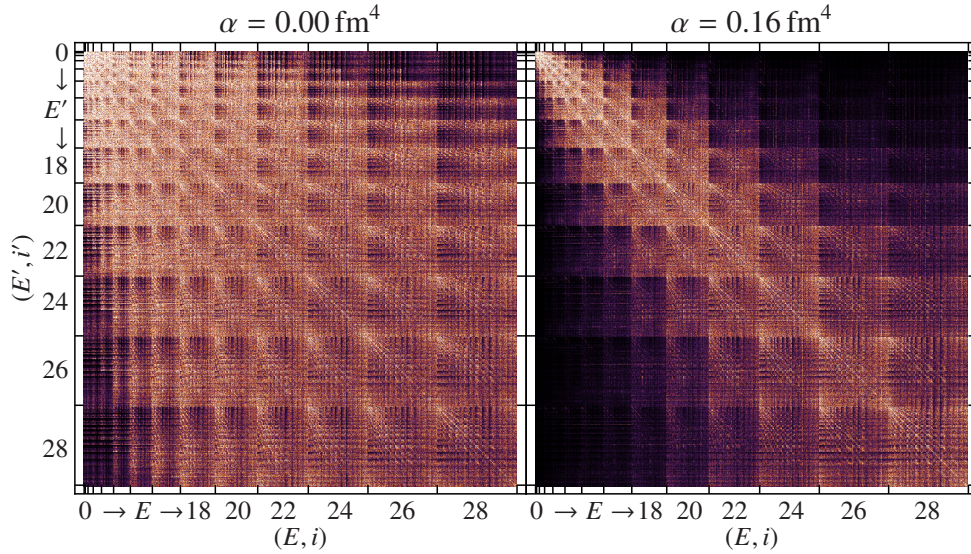
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Figure 1: Effect of the SRG evolution on the matrix elements of the NN+3N-full interaction in a three-body harmonic-oscillator Jacobi basis for $J^\pi = 1/2^+$ and $T = 1/2$ and oscillator frequency $\hbar\Omega = 28$ MeV. Plotted are the absolute values of the matrix elements. Light colors represent large values and dark colors represent values near zero.

the computational cost tremendously. Recently, this NO2B approximation has been successfully applied also in the (Multi-Reference) In-Medium SRG approach, which is a new ab initio method capable of studying closed- and open-shell nuclei alike [16, 17].

Finally, chiral NN+3N interactions can be employed and benchmarked in ab initio nuclear reaction theories, which give access to a wealth of scattering and reaction observables. To this end we have, for the first time, included explicit 3N interactions into the framework of NCSM combined with the Resonating Group Method (NCSM/RGM), see [18] for first results.

2. Similarity Renormalization Group with 3N Interactions

The Similarity Renormalization Group (SRG) is one of the most flexible and still simple methods to unitarily evolve the Hamiltonian towards a band-diagonal form with respect to a chosen uncorrelated many-body basis. The continuous unitary transformation or evolution of the Hamiltonian is governed by the flow equation

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} H_\alpha = [\eta_\alpha, H_\alpha], \qquad \eta_\alpha = (2\mu)^2 [T_\mathrm{int}, H_\alpha] = -\eta_\alpha^\dagger , \tag{2.1}$$

with η_α as dynamic generator of the transformation. Note that this generator itself depends on the continuous flow parameter α. In order to obtain the transformed Hamiltonian (or other consistently transformed observables, e.g. electromagnetic multipole operators or radii), one has to solve a first-order differential equation, which is a rather simple task. The flexibility of the SRG results from the fact that one can design the generator at will as long as it is antihermitian. In the following we restrict ourselves to a generator defined as commutator of the intrinsic kinetic energy T_int and

the evolved Hamiltonian, which is the standard choice in the context of nuclear physics, see for example [19]. However, other choices of the generator are possible and under investigation.

We solve the operator equation (2.1) by conversion into a matrix-element representation with respect to a *n*-body basis. Technically, this results in a system of coupled ordinary differential equations for the matrix elements of the transformed Hamiltonian H_α, which can be solved using standard Runge-Kutta methods. The effect of the SRG transformation on the matrix elements of the NN+3N interaction in the harmonic-oscillator Jacobi basis is depicted in Figure 1. In the left-hand panel we show the initial interaction, i.e., $\alpha = 0.0\,\text{fm}^4$. The matrix contains matrix elements with large absolute values even far off the diagonal. The right-hand panel shows the SRG-transformed matrix for flow parameter $\alpha = 0.16\,\text{fm}^4$. Clearly, the SRG yields the desired pre-diagonalization of the matrix and thus a decoupling of low- and high-energy degrees of freedom.

By representing the Fock-space operator equation (2.1) in an *n*-body basis, i.e., by projecting it into the *n*-body Hilbert space, SRG-induced operator contributions beyond the *n*-body level are discarded. Presently, we can account for all many-body contributions up to the three-body level, i.e., we are able to include all two- and three-body terms of the evolved Hamiltonian. We can define three different SRG-evolved Hamiltonians that will be used for the many-body calculations later on: *(i) NN-only*: start with an initial NN interaction and keep the two-body terms only; *(ii) NN+3N-induced*: start with an initial NN interaction and keep two- and induced three-body terms; *(iii) NN+3N-full*: start with an initial NN+3N interaction and keep the two- and all three-body terms.

At present, we have to omit all four- and higher-order many-body forces, which are induced by the unitary flow. This truncation formally violates the unitary character of the SRG. To assess the relevance of these neglected contributions we can investigate the dependence of the eigenvalues of the Hamiltonian (or any other observable) on the SRG flow parameter α. If omitted many-body forces are important, we will detect it through an α-dependence of the energy eigenvalues.

3. Importance Truncated No-Core Shell Model

We can now apply the SRG-transformed chiral NN+3N interactions in nuclear-structure calculations for nuclei throughout the *p*- and lower *sd*-shell. To solve the eigenvalue problem of the Hamiltonian, we employ the Importance Truncated No-Core Shell Model (IT-NCSM), which was developed in our group [11, 12]. The underlying idea is simple: for the description of a limited set of low-energy target eigenstates not all the basis states of the $N_{\max}\hbar\Omega$ model space of the NCSM are relevant. By means of an *a priori* importance measure derived from many-body perturbation theory we can assess the importance of each individual basis determinant. All basis states with importance measures below a specific threshold are discarded, and consequently the dimension of the matrix eigenvalue problem is reduced. Nevertheless, after a set of IT-NCSM calculations for a sequence of threshold values we can recover the full NCSM results with an *a posteriori* extrapolation of all desired observables to vanishing threshold [12]. Therefore, the IT-NCSM gives access to all observables tractable in the full NCSM with controlled and quantified uncertainties resulting from the threshold extrapolation. However, the range of nuclei and model-space sizes within computational reach of the IT-NCSM is significantly expanded compared to the full NCSM.
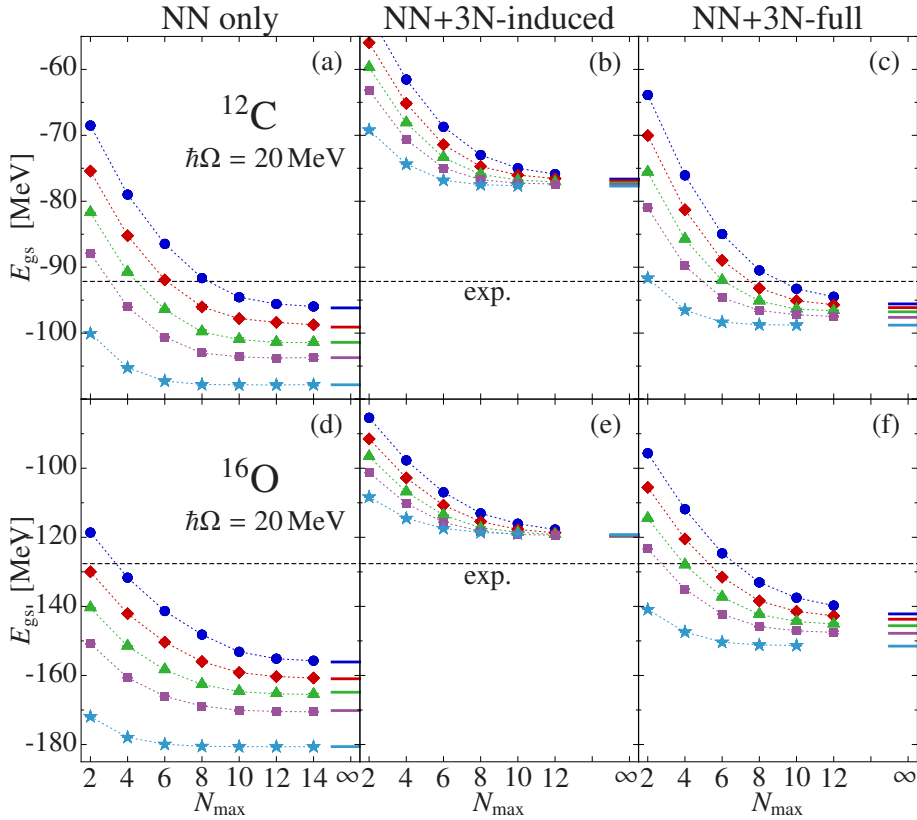
Figure 2:   IT-NCSM ground-state energies for ^{12}C and ^{16}O as function of $N_{\max}$ for the three types of Hamiltonians (see column headings) for a set of flow parameters: $\alpha = 0.04\,\mathrm{fm}^4$ (●), $0.05\,\mathrm{fm}^4$ (◆), $0.0625\,\mathrm{fm}^4$ (▲), and $0.08\,\mathrm{fm}^4$ (■), and $0.16\,\mathrm{fm}^4$ (★). Taken from Ref. [20].

Furthermore, starting from harmonic-oscillator Jacobi matrix elements of the 3N interaction we have developed a new approach for handling the 3N matrix elements, based on a memory-optimized *JT*-coupled storage scheme. Throughout the many-body calculation we take advantage of an efficient on-the-fly decoupling of these matrix elements, which eventually may be evaluated even on graphics processing units [21]. It turned out that this new scheme is the key for the inclusion of 3N forces in huge model spaces, in particular for nuclei in the upper *p*-shell and beyond [22], and for the CC and NCSM/RGM calculations mentioned above.

In Figure 2 we show ground-state energies obtained from IT-NCSM calculations for ^{12}C and ^{16}O for a set of flow parameters α as function of the model-space size $N_{\max}$. Due to the importance truncation and the new handling of 3N matrix elements we are able to treat $N_{\max} = 12$ model spaces, which is sufficient to obtain converged ground-state energies for the soft interactions. The left-hand panel shows our results using the NN-only Hamiltonian, i.e., without any 3N terms, which are afflicted with a strong dependence on the SRG flow parameter. This behavior hints at relevant, omitted induced 3N forces. If we include them consistently using the NN+3N-induced Hamiltonian, as shown in the middle panel, the α-dependence vanishes. This means the higher-order many-body forces induced from the initial two-body force are irrelevant. The resulting ground states are less bound compared to the NN-only results and can be seen as the true answer for the
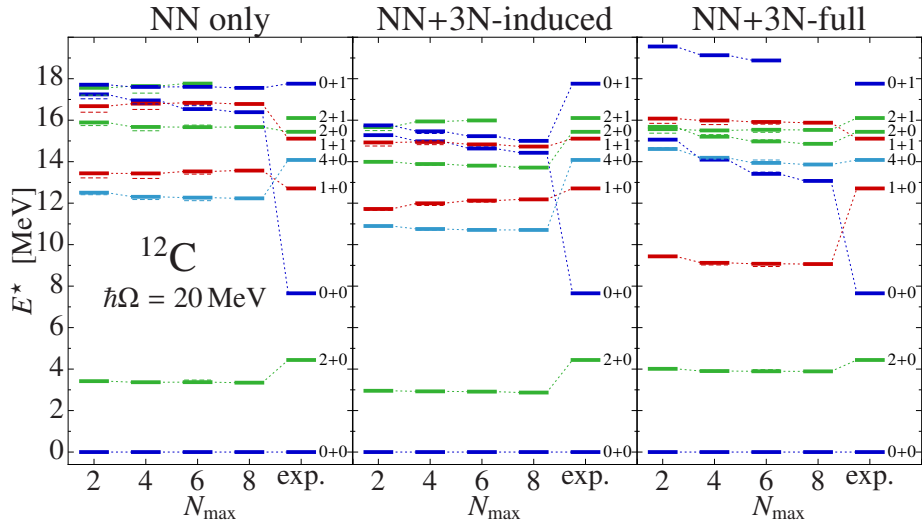
Figure 3: Excitation spectrum for the lowest positive-parity states (labelled $J\pi T$) in ^{12}C for the NN-only, the NN+3N-induced, and the NN+3N-full Hamiltonian with $\alpha = 0.08\,\text{fm}^4$. The thin dashed bars (mostly hidden) show results for $\alpha = 0.0625\,\text{fm}^4$. Taken from Ref. [20].

initial chiral NN force. The right-hand panel shows the results from the NN+3N-full Hamiltonian, i.e., including the initial chiral 3N interaction, with a re-emergence of the α-dependence of the ground-state energies. Thus, omitted 4N contributions that are induced during the SRG transformation with the initial 3N interaction have sizable effects on the ground-state energies of nuclei beyond the lower p-shell [20, 14].

The impact of the SRG-induced 4N interactions depends on the observable—for excitation energies it is much weaker. This is illustrated in Figure 3 for the excitation spectrum of ^{12}C computed with the three different Hamiltonians for two different SRG parameters. Once the spectra are converged with respect to model-space size, they do not show a significant dependence on α. Therefore, predictions using the chiral NN+3N forces and their validation against experiment are possible for excitation spectra and spectroscopic observables, even without the inclusion of SRG-induced 4N forces.

4. Sensitivity Analysis

Based on the developments discussed above, we are able to study the sensitivity of nuclear structure observables on the inputs from chiral EFT. In a first investigation we limit ourselves to excitation energies of p-shell nuclei as observables and the LECs and the cutoff of the chiral 3N interaction at N^{2}LO as input parameters. Eventually, these sensitivity studies aim at a consistent uncertainty propagation from the chiral EFT inputs to nuclear observables. These sensitivity analyses will also provide direct feedback for the construction of chiral EFT interaction, e.g., regarding the relevance of individual diagrams and operator structures in the chiral expansion or the impact of error bands for individual LECs on nuclear structure observables. They will provide guidance,
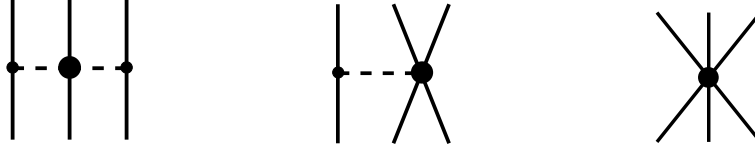
Figure 4: 3N diagrams at next-to-next-to leading order chiral perturbation theory. Solid and dashed lines represent nucleons and pions respectively.

e.g., for a selective inclusion of higher-order contributions of the chiral expansion or for targeted improvements of error bands for the most relevant LECs.

The diagrams of the leading order chiral 3N interactions are a two-pion exchange (TPE), a two-nucleon contact one-pion exchange and a three-nucleon contact, as depicted in Figure 4. The corresponding operator structures are

$$\sum_{i \neq j \neq k} \frac{1}{2} \left(\frac{g_A}{2F_\pi} \right)^2 \frac{(\vec{\sigma}_i \cdot \vec{q}_i)(\vec{\sigma}_j \cdot \vec{q}_j)}{(\vec{q}_i^2 + M_\pi^2)(\vec{q}_j^2 + M_\pi^2)} F_{ijk}^{\alpha\beta} \tau_i^\alpha \tau_j^\beta$$

$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta} \left[-\frac{4c_1 M_\pi^2}{F_\pi^2} + \frac{2c_3}{F_\pi^2} \vec{q}_i \cdot \vec{q}_j \right] + \sum_\gamma \frac{c_4}{F_\pi^2} \varepsilon^{\alpha\beta\gamma} \tau_k^\gamma \vec{\sigma}_k \cdot [\vec{q}_i \times \vec{q}_j] \tag{4.1}$$

for the two-pion exchange diagram with LECs c_1, c_3 and c_4,

$$- c_D \sum_{i \neq j \neq k} \frac{g_A}{8F_\pi^4 \Lambda_\chi} \frac{\vec{\sigma}_j \cdot \vec{q}_j}{\vec{q}_j^2 + M_\pi^2} (\vec{\tau}_i \cdot \vec{\tau}_j)(\vec{\sigma}_i \cdot \vec{q}_j) \tag{4.2}$$

for the two-nucleon contact one-pion exchange diagram with LEC c_D, and

$$c_E \sum_{j \neq k} \frac{1}{2F_\pi^4 \Lambda_\chi} (\vec{\tau}_j \cdot \vec{\tau}_k) \tag{4.3}$$

for the three-nucleon contact diagram with LEC c_E [23, 3]. The LECs c_i accompanying the pion-nucleon vertices already appear in the NN potential. However, in the literature exist various sets of possible values for these c_i constants, see e.g. [1, 24, 25, 26, 27], which have sizable deviations from each other. These different choices for the LECs will affect the predictions of nuclear structure observables obtained with the chiral 3N interactions.

In addition to these uncertainties, selected diagrams of the 3N interaction at N^{3}LO can be absorbed into the operator structures at N^{2}LO by simply shifting the values of the c_is by about 20-30%, for details see Ref. [5, 28]. In order to study the sensitivity of nuclear structure observables on these shifts and the different operator structures we adopt the c_i-shifts suggested in Ref. [28]. Note that the LECs entering the NN interaction remain unchanged. For the LEC c_D we stick to $c_D = -0.2$ as in the standard Hamiltonian, which warrants the reproduction of the β-decay half-life [29]. Finally, we fit c_E to the ground-state energy of ^{4}He at the bare interaction level. Then, this Hamiltonian, which still is fixed entirely in the three- and four-body system, is evolved consistently in the SRG framework and enters into the IT-NCSM calculations.

In Figure 5 we illustrate the dependence of the ^{12}C excitation spectrum on the different c_i-shifts. For comparison, we include in the first and second column the excitation energies obtained
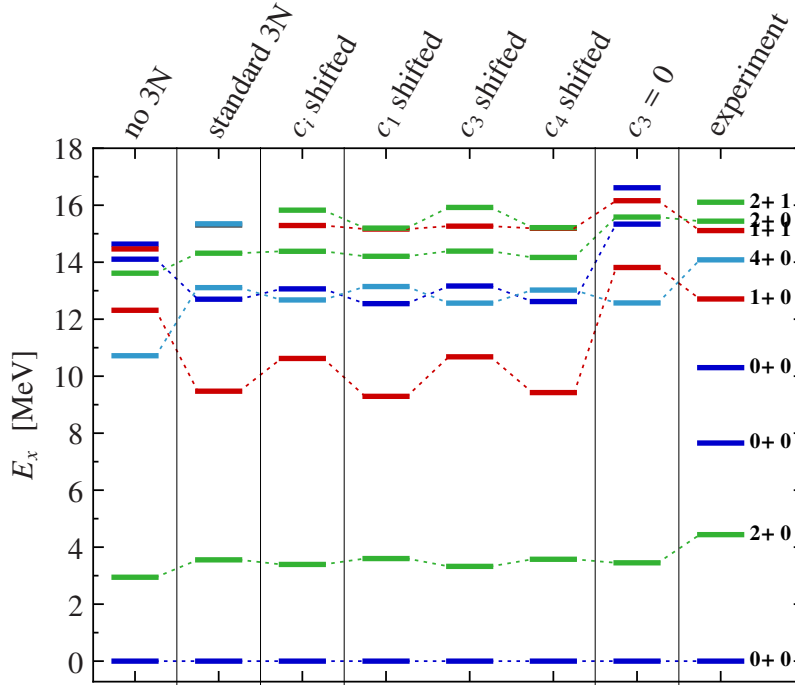
Figure 5: Sensitivity of the excitation spectrum of ^{12}C on the low-energy constants c_i. For a detailed explanation of the column headings see text. The IT-NCSM model space has been truncated at $N_{max} = 8$, the HO frequency is $\hbar\Omega = 16\,\text{MeV}$ and the SRG flow parameter $\alpha = 0.08\,\text{fm}^4$. Experimental data taken from [30].

from calculations with the NN+3N-induced and standard NN+3N-full Hamiltonian, respectively. The third column shows the spectrum corresponding to the 3N interaction using the shifted values for c_1, c_3 and c_4, i.e., effectively including some TPE topologies from N^{3}LO. We find most of the excitation energies rather insensitive to the changes in the LECs. The only exception is the first 1^+ state—its excitation energy is changed significantly by the c_i-shifts. The question whether this change is induced by all the c_i shifts or just by a subset of them is answered through the spectra shown in columns four to six, where only a single c_i has been shifted while the remaining LECs are kept at their original values. The shift of c_1 does not affect the excitation spectrum and, in particular, not the first 1^+ state compared to the standard 3N Hamiltonian. The same is true for the shift in c_4. In contrast, the shift of c_3 moves the excitation energy of the first 1^+ state by about the same amount as in the case where all c_i constants have been shifted simultaneously. In conclusion, the c_3-term has a direct and strong impact on the first 1^+ state, whereas other states rather robust under variations of c_3 and the other c_i. The important role of c_3 is confirmed next-to-last column of Figure 5 which depicts the ^{12}C spectrum for $c_3 = 0$. While the lowest 2^+ and 4^+ states remain insensitive, the first 1^+ state changes dramatically and also several high-lying excitations are effected.

Using the same procedure we can extend the sensitivity analysis to the remaining LEC c_D in Eq. (4.2) or to the 3N cutoff Λ. In the second to fourth columns of Figure 6 we show the ^{12}C
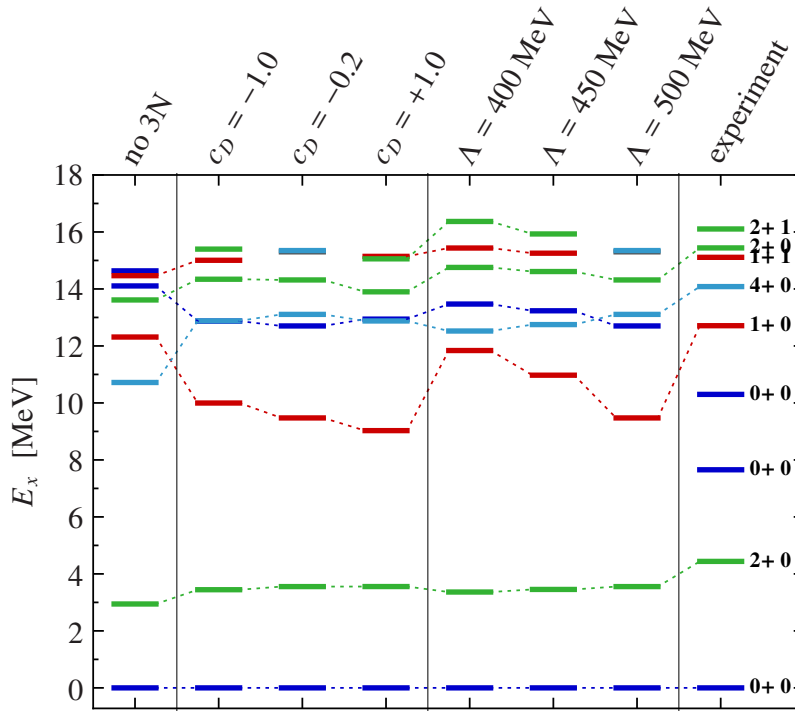
Figure 6: Sensitivity of the excitation spectrum of ^{12}C on the low-energy constant c_D and on variations of the 3N cutoff Λ. For a detailed explanation of the column headings see text. The IT-NCSM model space has been truncated at $N_{max} = 8$, the HO frequency is $\hbar\Omega = 16\,\text{MeV}$ and the SRG flow parameter $\alpha = 0.08\,\text{fm}^4$. Experimental data taken from [30].

spectrum obtained with $c_D = -1$, $c_D = -0.2$ (standard value) and $c_D = +1$, respectively. Again, we refit c_E to the binding energy of ^{4}He. Most of the states are rather insensitive to the variations of c_D, again with the exception of the first 1^+ state which is influenced most. The findings are similar for variations of the cutoff of the 3N interaction, as shown in the three next-to-last columns for $\Lambda = 400, 450$ and $500\,\text{MeV}$, respectively. Most of the excitation energies show only small changes, but the excitation energy of the first 1^+ state is significantly reduced with increasing cutoff.

We find a similar behavior as for the first 1^+ state in ^{12}C also for the lowest 1^+ state in ^{10}B. The sensitivity study with respect to the c_i values reveals that c_3 is crucial for obtaining the correct ground state. In Figure 7 we present the excitation energy of the first 1^+ state in ^{12}C in a correlation plot versus the energy difference between the first 3^+ and the 1^+ state of ^{10}B. Each point in the correlation plot corresponds to a different Hamiltonian, i.e., a different choice of the LECs or cutoff. All data points cluster along a single line, which is clearly separated from the experimental point. Consequently, within the scope of parameter variations discussed here, it is not possible to get the excitation energies of the lowest 1^+ states in ^{12}C and ^{10}B into agreement with experiment simultaneously. This may hint at missing operator structures in the initial chiral Hamiltonian. Additional operator structures could arise either from sub-leading 3N interactions, i.e., from higher orders in chiral perturbation theory, or from explicit considerations of the Δ excitation as degree of freedom in the EFT.
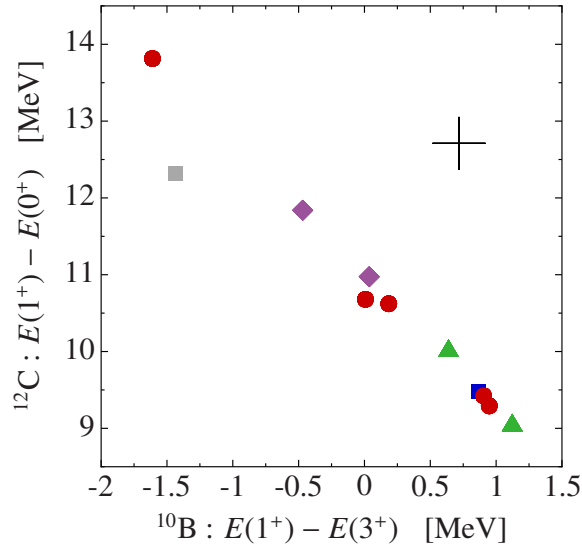
Figure 7: Correlation between the excitation energy of the first 1^+ state of ^{12}C and the energy difference between the first 1^+ and 3^+ states of ^{10}B. The cross marks the experimental point. The colored symbols correspond to (■) calculations without 3N interaction, (■) results obtained with the standard NN+3N-full Hamiltonian, (●) c_i variations, (▲) variations of c_D, and (◆) 3N cutoff variations.

5. Conclusions

We have discussed our recent progress regarding the consistent SRG-transformation of NN+3N Hamiltonians, the key developments concerning the handling of matrix-elements of 3N forces, and their use in the IT-NCSM approach for ab initio studies with chiral NN+3N interactions. This paves the way for extensive studies of the spectroscopy of p- and sd-shell nuclei. We have shown the relevance of SRG induced four- and higher-body interactions in case of absolute energies for nuclei in the upper p- and sd-shell. On the other hand we have observed that the effects of these induced forces are small for relative energies, i.e., excitation spectra. This allows for first sensitivity studies of the low-lying spectra of ^{12}C and ^{10}B with respect to details of the chiral 3N interactions, e.g. low-energy constants and the 3N cutoff. We have observed the important role of the c_3-term in the chiral 3N interaction for the correct description of certain states in p-shell nuclei, in particular the ground state of ^{10}B. Furthermore, these first studies hint at deficiencies, i.e., missing operator structures, in the leading chiral 3N interactions and provide further motivation to include the sub-leading contributions to the chiral 3N interaction.

The developments discussed here together with the progress, e.g., for medium-mass nuclei based on CC and for reactions and scattering of light nuclei within the NCSM/RGM approach—all including explicit 3N interactions—establish a path from low-energy QCD to nuclear structure and reactions observables through chiral effective field theory.

Acknowledgements

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