Invited Comment

Emergent properties of nuclei from *ab initio* coupled-cluster calculations*

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Abstract

Emergent properties such as nuclear saturation and deformation, and the effects on shell structure due to the proximity of the scattering continuum and particle decay channels are fascinating phenomena in atomic nuclei. In recent years, *ab initio* approaches to nuclei have taken the first steps towards tackling the computational challenge of describing these phenomena from Hamiltonians with microscopic degrees of freedom. This endeavor is now possible due to ideas from effective field theories, novel optimization strategies for nuclear interactions, *ab initio* methods exhibiting a soft scaling with mass number, and ever-increasing computational power. This paper reviews some of the recent accomplishments. We also present new results. The recently optimized chiral interaction NNLO\(^{sa}\) is shown to provide an accurate description of both charge radii and binding energies in selected light- and medium-mass nuclei up to \(^{56}\)Ni. We derive an efficient scheme for including continuum effects in coupled-cluster computations of nuclei based on chiral nucleon–nucleon and three-nucleon forces, and present new results for unbound states in the neutron-rich isotopes of oxygen and calcium. The coupling to the continuum impacts the energies of the \(J^p = 1/2^-, 3/2^-, 7/2^-, 3/2^+\) states in \(^{17,23,25}\)O, and—contrary to naive shell-model expectations—the level ordering of the \(J^p = 3/2^+, 5/2^+, 9/2^+\) states in \(^{53,55,61}\)Ca.

Keywords: *ab initio* computations of nuclei, saturation, effects of continuum on unbound states, deformation

(Some figures may appear in colour only in the online journal)

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Atomic nuclei exhibit a variety of fascinating phenomena that—on a microscopic level—range from single-nucleon motion to the collective behavior of practically all nucleons [1, 2]. Many of these can be viewed as emergent phenomena, that is, they are very difficult to derive from (or to understand from) the underlying microscopic Hamiltonian since they differ in scale and complexity from the fundamental constituents. Here we broadly understand emergent properties as proposed by Anderson [3]: ‘the ability to reduce everything to simple
fundamental laws does not imply the ability to start from those laws and reconstruct the Universe...at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other’.

In the physics of atomic nuclei, we mention the following examples of emergent phenomena: the long-range part of the nuclear interaction results from pion exchange and is thus a consequence of the spontaneous breaking of chiral symmetry in quantum chromodynamics (QCD). Rotations are the lowest excited states in rare Earth nuclei and actinides, as a consequence of the emergent breaking of rotational symmetry [4]. Pairing and nuclear superfluidity [5] results from the emergent breaking of a unitary symmetry. In neutron-rich nuclei with ground states close to the breakup thresholds, the interplay between pairing effects and the coupling to the particle decay channels may cause Borromean properties and extended halo-like density distributions to emerge [6–8]. Furthermore, the finely tuned saturation of atomic nuclei as self-bound finite quantum systems with an approximately constant density can also be viewed as an emergent phenomenon. Indeed, an inspection of the nucleon–nucleon interaction would not suggest that nuclear matter saturates, but repulsive three-nucleon forces (3NFs) combined with attractive nucleon–nucleon interactions achieve the feat [9–11]. In this article, we also consider phenomena that emerge in neutron-rich nuclei because these are inherently open quantum many-body systems with a strong coupling to the particle continuum and decay channels. Weakly bound and unbound states are most fascinating properties in neutron-rich nuclei, with surprising effects on binding and shell structure.

These examples show that much of the rich structure of atomic nuclei is due to emergent phenomena. Not surprisingly, the microscopic understanding of emergent phenomena poses significant theoretical challenges. We note that emergent phenomena are usually collective in nature and complex at the microscopic level. As a consequence, the corresponding emergent properties (such as the values for the pion mass, nuclear moments of inertia, nuclear pairing gaps, the nuclear saturation energy and density, the properties of halo states for the examples given in the previous paragraph) are usually finely tuned and cannot be guessed from the ‘natural’ sizes of the parameters of the underlying microscopic Hamiltonians.

Let us briefly comment on the microscopic approaches to emergent phenomena in nuclear physics. Lattice QCD calculations are now reaching physical pion masses for certain observables [12–14]. However, there is disagreement whether nuclear binding increases [15, 16] or decreases [17] with increasing pion mass. First ab initio computations of rotational bands in p-shell and sd-shell nuclei have become available very recently [18–22]. Here, the reproduction of moments of inertia for certain deformed sd-shell nuclei is very encouraging, while the accurate computation of transition strengths from first principles is still an open problem. Ab initio computations of superfluid properties have also been reported recently for nuclei in the oxygen and calcium region [23, 24]. Here, the accurate reproduction of pairing gaps and the restoration of particle number are challenges. Regarding nuclear saturation, only very few nuclear interactions yield accurate binding energies and radii for light [25] and medium-mass nuclei [11] that are also consistent with the empirical saturation point in nuclear matter. In nuclei heavier than oxygen or so, there seems to be a tremendous sensitivity to details of the nuclear interaction that are not probed in few-nucleon systems. Finally, the inclusion of continuum effects is essential for the level ordering of weakly bound and unbound states [26, 27], and the neutron dripline in exotic nuclei.

Let us also attempt to give a meaningful definition of accuracy in ab initio computations. Green’s function Monte Carlo methods computed energy levels of light nuclei to within 2% accuracy when compared with data [28]. Reference [29] lists a number of heavier nuclei for which binding energies fall within 5% of data, and a similar accuracy is possible for radii. In this paper, we refer to such calculations as being accurate.

The microscopic approach to emergent nuclear phenomena has become possible due to advances in computational nuclear physics. Chiral effective field theory (EFT), for instance, provides us with interactions that are consistent with the physics of low-energy QCD, and the pion mass and pion-nucleon interaction is taken from data [30–33]. Collective models [4, 34] and EFTs of heavy atomic nuclei [35–37] are based on bosonic degrees of freedom, with moments of inertia (or vibrational frequencies) as input parameters and low-energy constants, respectively. Finally, saturation is built into the nuclear shell model by tuning the frequency of the oscillator basis accordingly [38, 39].

The purpose of this article is to review and discuss recent and new results on emergent phenomena that now can be approached in ab initio coupled-cluster computations of atomic nuclei. The article is organized as follows. First, we give a brief theoretical background. Second, we discuss how nuclear saturation can be viewed as an emergent property and present the current status of accurate calculations of nuclear binding energies and radii from chiral interactions. Third, we discuss how simple and new patterns of shell-structure emerge in neutron-rich oxygen and calcium isotopes from complex many-body computations in which effects of both coupling to the particle continuum and the inclusion of 3NFs are significant. Fourth, we discuss how to construct non-perturbative shell-model interactions from coupled-cluster theory starting from nucleon–nucleon and 3NFs. Using standard shell-model tools we can describe the emergence of rotational bands from first principles. Finally, we discuss future perspectives and some of the challenges that we might expect when extending the nuclear coupled-cluster program beyond its current reach.

1. Theoretical background

The coupled-cluster method was introduced in nuclear physics in the late 1950s by Coester and Kümmerl [40, 41]. Shortly thereafter it sparked in quantum chemistry when Čižek introduced it in the 1960s as a tool to study correlated
in many-electron systems [42, 43]. In quantum chemistry it then quickly became the method of choice for solving many-electron problems. In nuclear physics on the other hand, it saw only sporadic applications in the first few decades after its inception [44–46]. During the last decade or so, coupled-cluster theory has been revitalized in nuclear physics [47–52] and has been used to compute nuclei from scratch based on modern forces from chiral EFT, see [53] for a recent review. Its role has also changed from being mostly post-dictive to having predictive capabilities. Examples are the prediction of the energy of the experiment to also having predictive capabilities. Examples of the dipole polarizability and the neutron distribution of $^{48}$Ca [29].

Let us briefly discuss some technical details of the coupled-cluster method and refer the reader to [56] for a comprehensive review. Coupled-cluster theory can be viewed as a (non-unitary) similarity transformation of the Hamiltonian such that the Hartree–Fock reference becomes an exact eigenstate in a Hilbert space limited to $n$-particle–$n$-hole ($np$–$nh$) excitations of the reference state. The similarity transformation is generated by the exponentiation of particle-hole excitation operators up to the $np$–$nh$ level. The workhorse is the coupled-cluster singles doubles (CCSD) approximation corresponding to $n = 2$, and triples $n = 3$ excitations are included perturbatively. The method has a polynomial cost in mass number and size of the single-particle basis, and Hartree–Fock references corresponding to closed (sub-)shell nuclei are computationally least expensive. The similarity-transformed Hamiltonian is at the center of the coupled-cluster method. Its diagonalization (via so-called 'equation-of-motion methods') in a Fock-space basis consisting of generalized particle-hole excitations yields excited states in the reference nucleus and states in neighboring nuclei that differ by one or two units in particle numbers or in the difference between neutron and proton numbers.

We perform coupled-cluster calculations based on the intrinsic Hamiltonian

$$
\hat{H} = \sum_{i<j} \left( \frac{(p_i - p_j)^2}{2m_A} + V^{(ij)}_{\text{NN}} \right) + \sum_{i<j<k} V^{(ijk)}_{\text{3N}},
$$

where $V^{\text{NN}}_{\text{NI}}$ is the nucleon–nucleon and $V_{\text{NI}}$ is the three-nucleon interaction. In coupled-cluster computations of nuclei the Hamiltonian enters in normal-ordered form, i.e.

$$
H_N = \sum_{pq} \langle p|f|q \rangle : a_p^\dagger a_q : + \frac{1}{4} \sum_{pqrs} \langle pq|v|rs \rangle : a_p^\dagger a_q^\dagger a_r a_s : + \frac{1}{36} \sum_{pqrsstu} \langle pqrs|w|stu \rangle : a_p^\dagger a_q^\dagger a_r^\dagger a_s^\dagger a_t a_u a_v :,
$$

with the normal-ordered string of creation and annihilation operators: $a_p^\dagger \ldots a_p^\dagger \ldots$. The normal-ordered one-body Fock matrix is

$$
\langle p|f|q \rangle = \langle p|\hat{n}|q \rangle + \sum_i \langle p|V^{\text{NN}}_{\text{NI}}|q \rangle_i + \frac{1}{2} \sum_{ij} \langle p|V^{\text{3N}}_{\text{NI}}|q \rangle_{ij},
$$

the normal-ordered two-body operator is given by

$$
\langle pq|v|rs \rangle = \langle pq|V^{\text{NN}}_{\text{NI}}|rs \rangle + \sum_i \langle pq|V^{\text{3N}}_{\text{NI}}|irs \rangle,
$$

and the normal-ordered three-body operator $w$ is given by

$$
\langle pqrs|w|stu \rangle = \langle pqrs|V^{\text{3N}}_{\text{NI}}|stu \rangle.
$$

Coupled-cluster calculations that include 3NFs are computationally very expensive [57, 58], and we therefore use the normal-ordered two-body approximation of the 3NF. This amounts to neglecting the residual three-body term given in equation (5). This approximation is accurate in light and medium mass nuclei [57–59].

We note that the coupled-cluster method preserves the translational invariance of the Hamiltonian to a large degree of accuracy, because the coupled-cluster wave function factors into an intrinsic wave function and a Gaussian center-of-mass wave function [51, 60, 61]. This property is not limited to the coupled-cluster method but is also demonstrated by other methods such as the in-medium similarity renormalization group (IMSRG) approach, see for example [22, 62].

2. Nuclear saturation

Atomic nuclei along the valley of $\beta$ stability are bound by about 8 MeV per nucleon, and charge radii scale approximately as $R_c \approx 1.2A^{1/3}$ fm, with $A$ denoting the mass number. The accurate computation of nuclear binding energies and radii from microscopic Hamiltonians has been a long-standing challenge in nuclear theory. For the light (p-shell) nuclei this challenge was successfully addressed by quantum Monte Carlo computations [25]. For interactions based on chiral EFT, radii and binding energies are well reproduced for light nuclei, while oxygen isotopes and heavier nuclei typically exhibit too much binding and too small radii, see [63, 64] for examples, and [11] for a compilation of results.

We note that nuclear saturation is a finely tuned property, and give several examples. Hebeler et al [10] considered families of similarity-renormalization group (SRG) transformed NN interactions [65] from chiral EFT with ‘bare’ 3NFs adjusted to the radii and binding energies of $^3$H and $^4$He. While the different interactions agree on the binding energy of the $^4$He nucleus within 1%, the corresponding Fermi momenta and binding energies at the saturation point of nuclear matter vary by about 10% and 25%, respectively. Likewise, Carlsson et al [66] found that different parametrizations of chiral EFT obtained from varying the chiral cutoff and the maximum nucleon–nucleon scattering energy used in the optimization, gives a spread in the binding energy of $^4$He of about 7%, while the corresponding spread in $^{16}$O is about 40%. In nuclear lattice EFT calculations based on chiral nucleon–nucleon and 3NFs, a repulsive phenomenological
We recall that the family of interactions from [10] differ in their high-momentum cutoff. This suggests that the saturation point in nuclear matter is sensitive to details of the chiral interaction. Consistent with this, coupled-cluster calculations of nuclear matter with interactions from chiral EFT showed that the saturation point is very sensitive to whether the employed high-momentum regulator functions are local or non-local [68]. On the one hand, these findings seem to be unexpected from the view of an EFT. After all, differences in high-momentum aspects are supposed to be higher-order effects in the chiral power counting. On the other hand, we remind the reader that the power counting is in the potential energy, and not in the total binding energy. Thus, it might be that variation in the binding energy is consistent with (3NF) interactions at N\(^2\)LO. Finally, we note that neutron matter is less sensitive to details of the high-momentum regulators [69, 70], presumably because only the two-pion exchange 3NF enters (for non-local regulators). For interactions from chiral EFT, the saturation mechanism consists of relatively soft NN forces that—taken alone—yield too much binding and too small radii. The 3NFs act repulsively in matter and heavier nuclei, playing thereby an important role in nuclear saturation [9–11].

Reference [68] also demonstrated that no adjustment of the short-range parts of the leading 3NFs is able to simultaneously reproduce the binding energy of \(^3\)H and the saturation point of nuclear matter (within a 5\% uncertainty). A similar result has been found for the Argonne V18 (AV18) NN interaction [71] and a family of 3NF models [72]. In [25, 73] it was also noted that AV18 with the Illinois 3NFs produce accurate results for binding energies and spectra of p-shell nuclei while less so for neutron matter. On the other hand, AV18 with the Urbana 3NFs produce good results for neutron matter while less accurate results for light p-shell nuclei.

In [11] this challenge was addressed by including data from ground-state energies and charge radii of \(^2\)H, \(^3\)H, \(^4\)He, \(^{12}\)C, \(^{16}\)O and ground-state energies of \(^{22,24}\)O into the optimization of the nuclear interaction NNLO\(_{\text{sat}}\) from chiral EFT at NNLO. Figure 1 shows the nuclei employed in the optimization as red stars on the Segrè chart. As a novelty, the NN and 3NF contributions of the chiral force NNLO\(_{\text{sat}}\) were also optimized simultaneously (and not sequentially). This approach is consistent with the inclusion of light nuclei into the optimization and with an adjustment of low-energy constants (LECs) order-by-order in the power counting. We refer the reader to [66] for a detailed comparison and discussion of sequentially and simultaneously optimized chiral interactions.

The inclusion of light nuclei beyond the three-nucleon bound states in the optimization of the nuclear interactions breaks with the traditional approach. There are additional arguments in support of this procedure. We note that the isospin \(T = 3/2\) component of the 3NF is not constrained by bound states in three- or four-nucleon systems. We also note that EFTs are concerned only with the description of low-energy data and observables [74]. It is therefore not necessary to limit the determination of LECs to the simplest systems imaginable. In EFTs of magnets, for instance, the relevant LECs are not determined in the two-body system but rather from bulk properties at low energies [75–77]. Finally, we note that the most accurate computations of light nuclei up to mass number \(A \leq 12\) [25] employ 3NFs that have been adjusted to 20 states in nuclei with mass numbers \(A \leq 10\) [25, 78]. Though they result from a non-perturbative solution of a quantum many-body problem, ground-state energies and charge radii of finite nuclei are truly low-energy observables.
and their inclusion in the optimization of LECs is thus consistent with EFT ideas. Reference [79] shows that the binding energies of $^3$H, $^4$He, and $^4$Li exhibit the same convergence pattern with increasing order of the chiral power counting as scattering observables at low energies of 10 MeV.

Figure 2 shows the results for ground-state energies per particle and differences between theoretical and experimental charge radii of selected light and medium-mass nuclei computed with NNLO$_{sat}$ and compares them to other ab initio computations. Here the results up to $^{40}$Ca are from [11], the results for $^{48}$Ca from [29], while the results for $^{56}$Ni are new. For the last two nuclei, the ground-state energy is computed using the CCSD with perturbative $\Lambda$-triples ($\Lambda$-CCSD(T)) [80], while for the lighter nuclei we also added a perturbative estimate for the residual 3NF term in equation (5) (yielding about 1% in additional binding energy). The computed binding energy per particle for $^{56}$Ni is 8.26 MeV slightly less than the experimental value of 8.64 MeV. The charge radius of $^{56}$Ni is not measured. Therefore we compare the computed charge radius of 3.72 fm to the known charge radius of $^{56}$Ni (which is probably larger than what is expected for $^{56}$Ni). The coupled-cluster calculations of $^{56}$Ni were performed in the same model space as [29]. We see that NNLO$_{sat}$ provides us with an improved description of the saturation properties in medium-mass nuclei.

Recently, Hagen et al [29] employed NNLO$_{sat}$ for the computation of the neutron density in $^{48}$Ca. The good agreement between theoretical results and data for the charge radii of $^{40,48}$Ca validated this approach, see figure 2. The radius $R_n$ of the point-neutron density was predicted as $3.47 \lesssim R_n \lesssim 3.60$ fm. Here, the theoretical uncertainties were estimated by correlating the theoretical results from NNLO$_{sat}$ and a family of chiral interactions [10] with the precisely known experimental charge radius. The strong correlation between the charge radii and point-neutron radii distinguishes ab initio results from nuclear density functional theory (DFT). As a consequence, ab initio results for the neutron skin, i.e. the difference between point-neutron and point-proton radii, exhibit almost no dependence of the employed chiral interaction. This is in contrast to results from nuclear DFT; the latter also exceed the former significantly.

As we have seen, chiral interactions with acceptable saturation properties have become available in recent years [10, 11], and they allow us to address burning questions in the physics of atomic nuclei. The extension of this program to even heavier nuclei is underway [90].

3. Continuum effects

Recently, efforts have been made in formulating an ab initio theory that unifies both structure and reactions in nuclei [91–96]. To describe reactions in nuclei one needs to account for decay channels in which coupling to both bound- and scattering states are important. The coupling to the continuum impacts also the level ordering of unbound states and shell-structure in nuclei. Understanding how shell structure evolve in neutron-rich nuclei is of great experimental and theoretical interest, in particular since shell structures impact the limits of stability known as the dripline (that is the limit where adding another neutron or proton to a bound isotope does not produce a particle stable ground-state), and thereby the number of nuclei that can exist. As the neutron-to-proton ratio varies it has been found in several isotopes that the magic numbers 2, 8, 20, 28, 50, … of the shell-model of Goeppert-Mayer and Jensen can be less magic than expected, while the appearance of new magic numbers in other isotopes have been observed. In this section we discuss and present new results for unbound states in the neutron-rich oxygen and calcium isotopes, with an emphasis on the role of coupling to the particle continuum and state-of-the-art chiral nucleon–nucleon and three-nucleon interactions.

3.1. Coupled-cluster calculations based on a Gamow–Hartree–Fock basis

As discussed in the previous section, coupled-cluster calculations based on chiral nucleon–nucleon and 3NFs can now accurately describe bulk properties such as binding energies and radii of light- and medium-mass nuclei. To provide experiment with reliable predictions for exotic nuclei, it is also necessary that the coupling to the scattering continuum is properly taken into account. Here we briefly outline and discuss how the coupling to the particle-continuum can be taken into account in ab initio coupled-cluster calculations of nuclei based on chiral nucleon–nucleon and 3NFs.

Similar to what is done in the Gamow-shell-model [97–99], we use a Berggren basis [100–102] as a starting point for our continuum coupled-cluster calculations [92, 103]. As depicted in figure 3 one can choose an appropriate contour $L'$ in the complex $k$-plane such that the usual completeness relation can be written as a discrete sum over bound- and resonant states and with an integral over the non-resonant...
continuum $L^+$ [104]. This is the Berggren completeness relation
\[
1 = \sum_{n \in \mathbb{N}} |\psi_n\rangle \langle \psi_n| + \int_{L^+} dk k^2 |\psi(k)| \langle \psi(k)|. \tag{6}
\]

In numerical applications the integral over $L^+$ is discretized using a suitable quadrature rule such as Gauss–Legendre, and converged results are usually obtained with $30–40$ quadrature points and a maximum real momentum of $\text{Re}[k] = 4.5$ fm$^{-1}$.

To obtain the Hamiltonian in the Berggren basis, $|a\rangle$, we utilize a finite expansion over harmonic oscillator states, $|\alpha\rangle$, i.e.
\[
\langle ab|V_{3N}|cd\rangle \approx \sum_{\alpha,\beta} \langle ab|\alpha\beta\rangle \langle \alpha\beta|V_{3N}|\gamma\delta\rangle \langle \gamma\delta|cd\rangle, \tag{7}
\]
which in the limit $n_{\text{max}} \to \infty$ is exact, while the kinetic energy is evaluated directly in the Berggren basis (see [92] for more details). We obtain a Gamow–Hartree–Fock basis [92, 105] by solving the Hartree–Fock equations in a mixed representation of harmonic-oscillator and Berggren basis states. This treats bound, scattering, and resonant states on an equal footing.

To construct a Gamow–Hartree–Fock basis starting from the Hamiltonian equation (1), the 3NF and the nucleon–nucleon interaction need to be represented in the Berggren basis. Generalizing the expansion given in equation (7) to include 3NFs is formally straightforward, but it represents a significant increase in the computational cost and memory. Below we show how a Gamow–Hartree–Fock basis can be computed efficiently. Let us start with the one-body Hartree–Fock Hamiltonian in the Berggren basis
\[
\langle \alpha|H_{1\text{F}}|e\rangle = \langle \alpha|\epsilon\rangle + \langle \alpha|V_{3N}|e\rangle + \langle \alpha|V_{3N}|e\rangle, \tag{8}
\]
consisting of a one-body kinetic energy term, and one-body potential terms arising from folding the nucleon–nucleon interaction and the 3NF with one-body density matrices, that is
\[
\langle \alpha|V_{3N}|e\rangle = \sum_{J} \sum_{pq} \left( \frac{2J + 1}{2J_a + 1} \right) \langle \alpha|p\rangle \langle q\rangle (|\epsilon|) \langle \epsilon|p\rangle, \tag{9}
\]
\[
\langle \alpha|V_{3N}|e\rangle = \frac{1}{2} \sum_{J} \sum_{pqrs} \left( \frac{2J + 1}{2J_a + 1} \right) \langle \alpha|pqrs\rangle \langle r\rangle \langle s\rangle \langle \rho\rangle \langle q\rangle. \tag{10}
\]

Note that $\langle \alpha|V_{3N}|e\rangle$ contains contributions from both the nucleon–nucleon interaction and from the two-body part of the intrinsic kinetic energy. The one-body density matrices $\langle \rho|\rho\rangle$ are constructed from the eigenvectors obtained by diagonalizing equation (8). The computation of $\langle \alpha|V_{3N}|e\rangle$ is expensive in the Berggren basis, however we can circumvent the problem of computing matrix elements of the 3NF directly in the Berggren basis by first writing
\[
\langle \alpha|V_{3N}|\gamma\delta\rangle = \frac{1}{2} \sum_{J} \sum_{pq} \sum_{\mu} \left( \frac{2J + 1}{2J_a + 1} \right) \langle \alpha|\mu\rangle \langle \nu\rangle \langle \gamma\delta\rangle \langle \mu\nu\rangle \langle \gamma\delta\rangle, \tag{11}
\]
Here, $\langle a|\alpha\rangle$ are radial overlap functions between a Berggren and a harmonic-oscillator basis state, and in the last term we introduced projections of the density matrices onto a finite harmonic-oscillator space, i.e.
\[
\langle \alpha|\rho\beta\rangle = \sum_{\alpha\beta} \langle \alpha|\alpha\rangle \langle \alpha|\beta\rangle \langle \beta|\beta\rangle. \tag{12}
\]
Finally, in order to obtain the one-body matrix elements $\langle \alpha|V_{3N}|e\rangle$, we introduce the expansion,
\[
\langle \alpha|V_{3N}|e\rangle = \sum_{\alpha\beta} \langle \alpha|\alpha\rangle \langle \alpha|V_{3N}|\beta\rangle \langle \beta|\beta\rangle. \tag{13}
\]
Using this strategy we can compute a Gamow–Hartree–Fock basis from nucleon–nucleon and 3NFs self-consistently by never having to represent the 3NF directly in the Berggren basis. The only requirement is that the one-body density matrices defined in the Berggren basis are projected onto a finite harmonic oscillator space after each Hartree–Fock iteration, then proceed by computing the 3NF contribution in equation (11), and finally projecting the $V_{3N}$ term onto the Berggren basis via equation (13). In practice one verifies that the results are converged with respect to the size of the finite harmonic oscillator space used. Once the Gamow–Hartree–Fock basis is self-consistently determined, the normal-ordered one- and two-body matrix elements given in equations (3) and (4) are evaluated in this basis.

3.2. Unbound states in neutron-rich oxygen isotopes

The oxygen isotopes have been extensively studied during the last decade. Here new (sub-) shell closures at $N = 14$ and $N = 16$ have been observed experimentally [106–108], while the $N = 20$ magic number is weakened and disappears along the isotope chain starting from $^{40}$Ca towards the island of inversion nuclei $^{32}$Mg and $^{36}$Ne, where the onset of large deformations is observed [109]. Furthermore, $^{24}$O is the last bound isotope with the ground-state of $^{25}$O being particle unstable at the neutron decay energy 770 keV and with a width of 172(30) keV [110]. This has become known as the oxygen anomaly, since by adding just one more proton pushes the neutron dripline considerably further out with $^{31}$F being the last known bound fluorine isotope [111]. This oxygen anomaly was given a theoretical explanation in [112], where it was shown in shell-model calculations that 3NFs act repulsively and correctly set the dripline at $^{24}$O. Perhaps even more interesting than $^{25}$O is its neighbor $^{26}$O. This nucleus has recently been observed at a decay energy of $150+50$ keV and with a width of 5 keV. It decays by two-neutron emission [113]. Few-body models of $^{26}$O have emphasized the role of di-neutron correlations in the two-neutron direct decay of this
The exotic nucleus $^{28}$O is close to the known island of inversion region, where intruder states from the pf-shell, deformation and continuum couplings play an important role for the structure of ground- and low-lying excited states [122, 123]. Furthermore, relativistic mean-field calculations of $^{25}$Ne found that the pf-orbitals are inverted due to continuum coupling even in the case of a spherical or slightly deformed $^{31}$Ne [122]. It is therefore reasonable to expect that configuration mixing from the pf-shell and continuum coupling will play a role on the structure of $^{28}$O as well. In order to cast some light on how important configuration mixing with the pf-shell may be on the structure of neutron-rich oxygen isotopes we study the evolution of the unbound $J^\pi = 1/2^-, 3/2^-, 7/2^-$ states and the unbound $J^\pi = 3/2^+$ state that are dominated by one-particle configurations in the odd oxygen isotopes $^{17,19}$O. These states can be computed in the particle-attached equation-of-motion coupled-cluster (PA-EOM-CC) method [124], and we include continuum effects by using a Berggren basis for the $d_{3/2}$, $p_{3/2}$, $p_{1/2}$ partial waves. The PA-EOM-CC method was previously used to compute resonances in $A = 17$ nuclei using nucleon–nucleon forces only [103], while here we for the first time we include also 3NFs and compute negative-parity states.

Figure 5 shows the energies of the unbound $J^\pi = 3/2^+$, $1/2^-$, $3/2^-$, $7/2^-$ states in the odd oxygen isotopes $^{17,19}$O using a harmonic-oscillator basis and a Berggren basis with respect to the particle-emission threshold. Here we only consider the chiral interaction $N^3LO + L(400)$, which is known to reproduce spectra in the sd-shell. It is seen that the effect of the continuum coupling on the $J^\pi = 3/2^+$ and $J^\pi = 7/2^-$ resonant states is rather small, which is due to
the large centrifugal barrier ($l = 2, 3$) for these states and that these states are dominated by one-particle radial wavefunctions of zero nodes, limiting thereby their radial extension and making them quasi-bound within the centrifugal barrier. On the other hand, the continuum coupling plays a significant role on the $J^p = 3/2^-, 1/2^-, 3/2^-$ and $7/2^-$ states in the odd oxygen isotopes $^{17,23,25}$O. For each nucleus the left group of states are computed using a harmonic-oscillator Hartree–Fock basis, while the corresponding right group states using a Gamow–Hartree–Fock basis. The role of continuum coupling on the individual states is indicated by the connecting dashed–dotted lines between the left and right group of states. The vertical bar on the right group of states gives the corresponding resonance width $\Gamma = −2\text{Im}[E]$ of each resonant state.

3.3. Unbound states in neutron-rich calcium isotopes

Recent interest in understanding how shell structures evolve in calcium isotopes has revealed several interesting and new features, such as the newly suggested magic nuclei $^{52}$Ca and $^{54}$Ca with $N = 32$ shell-closure [126], and $N = 34$ (sub-) shell-closure [54, 55]. While 3NFs have been shown to be important to explain these new (sub-) shell-closures [26, 127], coupled-cluster calculations of the odd and neutron-rich isotopes $^{53,55,61}$Ca [26] based on chiral nucleon–nucleon and schematic density-dependent 3NFs, demonstrated that the role of the coupling to the particle continuum significantly impacts and rearranges the order of states close to the particle-emission thresholds. In particular, for the exotic nucleus $^{64}$Ca the ground-state was computed to be a $J^p = 1/2^+$ state dominated by configurations in the $s$-partial-wave, and with a compressed and inverted order for the $J^p = 5/2^+, 9/2^+$ excited states in contrast to what one could expect from the standard shell-model. In [128] coupled-cluster computations of elastic neutron scattering on $^{60}$Ca were performed, and the extracted scattering length for the $s$-wave phase-shifts was found to be tens of fermi. The very large scattering length was used as input to halo EFT [129, 130] in order to explore the possible onset of Efimov physics in $^{62}$Ca.

The ‘bunching’ of the gds shell-model states in neutron-rich calcium isotopes has also been observed in nuclear density-functional and relativistic mean-field calculations, suggesting an onset of deformation around $^{60}$Ca and with the dripline possibly extending all the way out to $^{70}$Ca [131–134]. In addition to effects of the coupling to the continuum, deformation has also been shown to impact and lead to a near degeneracy of shell-model states in neutron-rich nuclei [135, 136]. Shell-model calculations based on phenomenological interactions also predicts a bunching and inversion of the $d_{5/2}$, $g_{9/2}$ shell-model orbitals in $^{56}$Ca [137]. Future experimental efforts at rare isotope facilities promise to probe shell structure beyond $^{54}$Ca. The heaviest calcium isotope to have been produced so far is $^{58}$Ca [138] and data on $^{62}$Ti is currently being analyzed at RIKEN. Confronting theory with data for the exotic nucleus $^{60}$Ca and beyond might therefore not be too far in the future.

In the remainder of this section we focus on the evolution of the $J^p = 3/2^+, 5/2^+, 9/2^+$ states in the odd calcium isotopes $^{34,55,61}$Ca. In these exotic isotopes there are no data for these states. We again use the PA-EOM-CC method to compute states that are dominated by one-particle excitations. Here we use the chiral nucleon–nucleon interaction at N$^3$LO [117], SRG evolved to the cutoff $\lambda = 1.8$ fm$^{-1}$. The low-energy constants of the leading-order chiral 3NF were adjusted to the binding energies and radii of $^4$He and $^6$He, and within systematic uncertainties reproduce the saturation point in nuclear matter [10]. This chiral interaction was recently applied to the computation of the binding energy, dipole polarizability, and the neutron/proton root-mean-square point radii of $^{48}$Ca [29]. For this interaction, $^{48}$Ca was found to be
slightly overbound by about 4 MeV while the charge radius was underestimated by about 0.2 fm. To construct a Gamow–Hartree–Fock basis, we use the same model space as in [29] (i.e. \(N_{\text{max}} = 14, E_{1\text{max}} = 16\) and \(\hbar\Omega = 22\) MeV), and a Berggren basis for the \(d_{3/2}, d_{5/2}, g_{9/2}\) partial waves.

Figure 6 shows the \(J^p = 3/2^+, 5/2^+, 9/2^+\) unbound states in the odd calcium isotopes \(^{53,55,61}\)Ca, computed in a Hartree–Fock basis built from harmonic oscillators only, and in a Gamow–Hartree–Fock basis. We observe a striking feature, the coupling to the continuum inverts the order of the \(J^p = 3/2^+, 5/2^+, 9/2^+\) states, with the \(J^p = 3/2^+\) state being a very broad resonance and with a decay energy located slightly above the decay energy of the \(J^p = 5/2^+\) resonant state, which has a considerable smaller width. Furthermore, in \(^{61}\)Ca we observe a near degeneracy for the decay energies of the \(J^p = 3/2^+, 5/2^+, 9/2^+\) states. We recall that in [128] the ground-state of \(^{61}\)Ca was found to be a barely bound \(J^p = 1/2^+\) state, dominated by \(s\)-waves. That the \(J^p = 3/2^+, 5/2^+, 9/2^+\) states are found to close to the threshold in \(^{61}\)Ca indicates that deformation and pairing will play a significant role in the neutron rich calcium isotopes beyond \(^{61}\)Ca. A proper theoretical description of isotopes beyond \(^{61}\)Ca should therefore account for all these effects, that is, continuum coupling, deformation and pairing, and many-body correlations.

In the naive shell-model picture one could expect that the \(J^p = 9/2^+\) state, which is dominated by \(g_{9/2}\) single-particle configurations, should be lower in energy than the \(J^p = 3/2^+, 5/2^+\) states, which are dominated by \(d_{3/2}, d_{5/2}\) single-particle configurations. As figure 6 shows, this naive shell-model order is in fact realized if one neglects the coupling to the particle-continuum and uses a harmonic-oscillator basis only. This result is consistent with what was found in [26, 128], where a schematic 3NF was used. We can understand the impact of the continuum on these unbound states by employing a simple mean-field picture. In this picture the \(J^p = 9/2^+\) state is a pure \(g_{9/2}\) single-particle state with a large centrifugal barrier \((l = 4)\). Furthermore, its wave-function has no radial nodes, localizing thereby the state within the barrier and making it quasi-bound. Indeed, as one would expect, figure 6 shows that the continuum has only a small impact on this state, lowering it by a few hundred keVs compared to the harmonic-oscillator basis, and with a width less than 10 keV. On the other hand, the continuum has a significant impact on the unbound \(J^p = 3/2^+, 5/2^+\) states. In the mean-field picture these states are pure \(d_{3/2}\) and \(d_{5/2}\) single-particle states with a smaller centrifugal barrier \((l = 2)\) and with wave-functions with one radial node that pushes these states outside the barrier. The impact of the continuum on these states is therefore significant, and similar to what was found for the \(J^p = 1/2^+, 3/2^+\) states in the oxygen isotopes \(^{17,23,29}\)O.

One may speculate that the trend found for unbound states in neutron-rich isotopes of oxygen and calcium may also be found in neutron-rich nickel isotopes. Here one may expect a level inversion of the unbound \(J^p = 11/2^+, 7/2^+\), \(3/2^-\) negative parity states associated with the \(0h1/2, 1f5/2, 2p3/2\) mean-field orbitals. Future experiments targeting spectroscopy in the exotic nuclei \(^{61}\)Ca and \(^{79}\)Ni is therefore needed in order to fully understand how shell-structure evolve at large neutron-to-proton ratios and above particle decay thresholds.

4. Emergence of nuclear deformation

Nuclear deformation is due to the emergent breaking of rotational symmetry, that is the precursors of spontaneous breaking of rotational symmetry in a finite system [1, 36, 139]. The key signatures are rotational bands with energies \(E \approx BI(l + 1)\) for states with angular momenta \(l = 0, 2, 4, \ldots\), and strong collective \(B(E2)\) transitions between these states. Here, the rotational constant \(B\) is typically much smaller than the energy scales associated with single-particle degrees of freedom [4]. The collective nature and the low energy of the emergent rotational constant \(B\) make \textit{ab initio} computations of such states challenging. For the nucleus like \(^{12}\)C, the energies of Yrast states were reproduced in the \textit{ab initio} computations detailed in [84, 85, 140, 141], with accurate quadrupole moments in [84]. Collective properties of other p-shell nuclei from \textit{ab initio} methods are addressed in [18, 20, 142]. Very recently, \textit{ab initio} computations of Yrast states in sd-shell nuclei have become possible [21, 22, 143]. These works are based on the recently developed effective shell-model interactions from \textit{ab initio} methods like coupled-cluster theory and IMSRG [120, 121].

The idea behind the coupled-cluster effective-interaction (CCEI) method is to compute a non-perturbative shell-model interaction using the coupled-cluster method and starting
from state-of-the-art chiral nucleon–nucleon interactions and 3NFs. In this approach, the coupled-cluster method is used to compute spectra in nuclei with one, and two nucleons outside a closed core [61, 124, 144, 145]. To be specific, the computation of neutron-rich isotopes of carbon and oxygen can be based on an effective neutron-interaction in the neutron sd-shell model space. Following [146, 147], ab initio computations of $^{14,15,16}$C and $^{16,17,18}$O are input to the Okubo–Lee–Suzuki projection technique [148–152], yielding an effective interaction in the neutron sd model space. The symmetric orthogonalization [153, 154] yields an effective interaction that is Hermitian. For each mass number one obtains a new interaction because the intrinsic kinetic energy of the underlying chiral Hamiltonian uses the mass number $A$ of the target nucleus. Without any further tuning of parameters, the CCEI method yields effective neutron–neutron interactions for oxygen and carbon isotopes with $^{16}$O and $^{14}$C as cores [121], respectively. The resulting spectra are in good agreement with experiment and comparable to the agreements obtained with phenomenological Hamiltonians such as the USD [38] and the WBP [155] effective shell-model Hamiltonians.

Recently, the CCEI has been extended to the full effective interaction between neutrons and protons in the sd-shell valence space, taking $^{16}$O as a core and performing $ab$ initio coupled-cluster calculations of $^{16,17,18}$O, $^{17,18}$F, and $^{18}$Ne. These calculations are based on the same chiral interaction used in [121], and the resulting effective shell-model interaction was again truncated to one-body and two-body terms. In contrast to [121], this effective shell-model interaction was constructed from a chiral interaction that uses the mass number $A$ of the $^{16,17,18}$O, $^{17,18}$F, and $^{18}$Ne nuclei. One obtains thereby an effective interaction for all sd-shell nuclei that is independent of the nucleon number $A$. Diagonalization of the resulting sd-shell Hamiltonian matrices allowed the authors of [21] to compute rotational bands of neon and magnesium isotopes.

Figure 7 shows the ground-state rotational bands in $^{20}$Ne and $^{24}$Mg and compares them to experimental data and to results from the USDB interaction [156]. The agreement of these yrast states to phenomenological interactions and data is good.

The computation of rotational bands (and the accurate reproduction of moments of inertia) are encouraging first results for $ab$ initio approaches to nuclear deformation. Our next steps will include the computation of static and transition electric quadrupole moments as well. The latter requires the development of effective (quadrupole) operators that are calculated within the same theoretical framework. Steps in these directions are under way and we expect that such approaches will result in new insights into the theory of effective charges.

5. Summary and outlook: simplicity from complexity

The physics of nuclei, with intricate forces yet to be completely determined, two different Fermionic species, many energy scales and the absence of an external potential, generates a range and diversity of behaviors that pose great challenges to a microscopic and predictive description. Computing and understanding the wide range of nuclear phenomena that emerge at different levels of complexity and energy scales from the underlying forces and laws of motion is still an open and unsettled issue. In the past decade, significant strides have been made toward this goal. The description of heavier nuclei using $ab$ initio approaches has now become possible due to recent development and advances in nuclear interactions, renormalization-group techniques, many-body methods and an increasing computing power that continues to scale according to Moore’s law.

Several many-body methods are now available that exhibit a polynomial scaling with mass number and are improvable in a systematic way [51, 63, 157–160]. This soft scaling combined with the exponential growth in computing power allows us now to address heavier nuclei from first principles for the first time. Modern nuclear forces, based on EFT concepts and ideas from renormalization group [32, 33, 161], and optimized to reproduce data on selected light nuclei yielded accurate results and even reliable predictions for a wide variety of nuclei [26, 112, 115, 126, 162]. An EFT interaction that was constrained to radii and binding energies of isotopes up to oxygen [11] accurately reproduced the charge densities in $^{40,48}$Ca and yielded a prediction of the neutron distribution of $^{48}$Ca [29]. The methodological advances in constructing single-particle and many-particle basis functions for continuum properties, allow us to study nuclei close to the limits of stability. Furthermore, as we illustrated here, we are now in a position where we can compute effective Hamiltonians (including single-particle energies and two-body interactions) for a single major shells. These effective interactions are without empirical adjustments and led to the computation of spectra of sd-shell nuclei. The onset of deformations in neon and magnesium isotopes were studied recently [21, 143] and reviewed in the previous section. These results demonstrate the potential and capabilities of present many-body methods.
Simple patterns in nuclei such as nuclear saturation, rotational and vibrational spectra, Borromean properties and halo-like density distributions properties, and shell-structure are now being approached from microscopic many-body calculations. We are reaching a point where few-body and mean-field models specifically aimed at describing such emergent phenomena can be complemented by more microscopic and refined models. This is not to say that these simpler models will be replaced by ever more complex and complicated quantum-mechanical many-body descriptions. They will continue to play an important role in the discovery process of new phenomena, and in their interpretation and understanding in terms of more intuitive pictures and ideas.

The microscopic description of nuclei from first principles highlights various aspects of the nuclear many-body problem, ranging from the optimization of low-energy constant of the nuclear interactions, the role of 3NFs, the role of high-momentum modes and many-body correlations, and to the treatment of the atomic nucleus as an open-quantum system with a strong coupling to the particle continuum and decay channels. Depending on the energy scales that are relevant for the description of the specific nuclear property and its origin, these components vary in their importance. For example, including the coupling to the particle continuum is not necessary for strongly bound nuclei, but it plays a crucial role on evolution of shell-structure in neutron-rich oxygen and calcium isotopes. Another example is the important role of 3NFs on nuclear saturation and on shell closures, while its role on ab initio calculations of rotational bands in the deformed nuclei \(^{20}\text{Ne}\) and \(^{24}\text{Mg}\) seems less prominent. Simple models of the nucleus may therefore often guide us in deciphering the importance of these different components.

We end this paper by pointing out several open challenges and exciting avenues. The recent work \cite{90} with interactions from EFT tailored to a harmonic oscillator basis, might hold some promise for performing accurate ab initio calculations for heavier nuclei and address issues related to nuclear shell-structure and saturation over the entire nuclear chart. The technical capabilities are now in place \cite{63}, and the onus is on the optimization of accurate interactions. Further development of open-shell methods such as CCEI and valence-space IM-SRG might open up a path for ab initio studies of neutrinoless double-beta decay in nuclei such as \(^{76}\text{Ge}\) and \(^{136}\text{Xe}\). Along similar lines, a derivation of effective operators and interactions for heavier nuclei opens up possibilities for studies of electroweak interactions in a nuclear medium.

These studies and the pertinent formalism can also be extended to infinite matter, of great interest for studies of dense objects like neutron stars. Reliable many-body derivations of the equation-of-state and effective interactions and operators for dense nuclear matter, are of great importance for far ranging issues like neutrino oscillations and the synthesis of the elements. Another topic which is of crucial importance for coming experimental programs is the link between the structure and the dynamics of nuclei, with topics like reactions in medium-mass nuclei and the derivation of for example optical potentials using present many-body methods.

Finally we would like to point out an unresolved challenge to our many-body methods. For any ab initio calculation to be truly meaningful, uncertainties at all levels of the calculation needs to be quantified. There are recent advancements in the quantification of systematic and statistical uncertainties of the employed Hamiltonian \cite{66,163,164} and of employing Bayesian statistics in nuclear EFTs \cite{37,165,167}. Propagation of these uncertainties from the underlying Hamiltonian to the nuclear many-body problem are underway \cite{168,169}. Besides uncertainties in the employed Hamiltonian, many-body methods such as coupled-cluster theory rely on an expansion using a finite single-particle basis. Finite basis truncations introduces another uncertainty which needs to be quantified. Recently formulas for infrared and ultraviolet extrapolations of binding energies, radii and quadrupole moments based on a harmonic oscillator basis in few- and many-body systems were derived \cite{170,177}. We also mention that for specific systems like quantum dots using effective interactions, precise error estimates for a given truncation of the harmonic oscillator basis may also be given, see for example \cite{178}. Finally, there is a systematic uncertainty related to the specific truncation of the applied many-body method. This uncertainty is perhaps the most challenging and difficult to address, with first steps made for the coupled-cluster truncation \cite{179,180}. Although most many-body methods are subject to systematic improvements and controlled approximations, a rigorous theory for the convergence with respect to truncation level is an unresolved and open problem.

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