Ab initio calculations of $p$-shell nuclei up to N$^2$LO in chiral Effective Field Theory

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Abstract. Nuclear structure and reaction theory are undergoing a major renaissance with advances in many-body methods, realistic interactions with greatly improved links to Quantum Chromodynamics, the advent of high performance computing, and improved computational algorithms. State-of-the-art two- and three-nucleon interactions obtained from chiral Effective Field Theory provide a theoretical foundation for nuclear theory with controlled approximations. With highly efficient numerical codes, tuned to the current generation of supercomputers, we can perform ab-initio nuclear structure calculations for a range of nuclei to a remarkable level of numerical accuracy, with quantifiable numerical uncertainties. Here we present an overview of recent results for No-Core Configuration Interaction calculations of $p$-shell nuclei using these chiral interactions up to next-to-next-to-leading order, including three-body forces. We show the dependence of the ground state energies on the chiral order; we also present excitation spectra for selected nuclei and compare the results with experimental data.

1. Ab Initio Nuclear Structure and High Performance Computing

A microscopic theory for the structure and reactions of atomic nuclei poses formidable challenges for high-performance computing. A nucleus with $Z$ protons and $N$ neutrons is a self-bound quantum many-body system with $A = N + Z$ strongly interacting nucleons. The interactions feature both attractive and repulsive contributions along with significant spin and angular momentum dependence. Furthermore there are both short-range and long-range terms in the interaction, and in addition to nucleon-nucleon (NN) interactions, one also needs suitable three-nucleon forces (3NFs), and possibly even higher many-body interactions. The corresponding Hamiltonian can be written as

$$\hat{H} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

(1)

where $m$ is the nucleon mass, which we take to be equal for protons and neutrons. The nuclear wave functions are the solutions of the many-body Schrödinger equation

$$\hat{H} \Psi(\vec{r}_1, \ldots, \vec{r}_A) = E \Psi(\vec{r}_1, \ldots, \vec{r}_A)$$

(2)

at discrete energy levels $E$.

In No-Core Configuration Interaction (NCCI) nuclear structure calculations [1] the wave function $\Psi$ of a nucleus consisting of $A$ nucleons is expanded in an $A$-body basis of Slater
determinants $\Phi_k$ of single-particle wave functions $\phi_{nljm}(\vec{r})$. Here, $n$ is the radial quantum number, $l$ the orbital motion, $j$ the total spin from orbital motion coupled to the intrinsic nucleon spin, and $m$ the spin-projection. The Hamiltonian $\hat{H}$ is also expressed in this basis and thus the many-body Schrödinger equation becomes a matrix eigenvalue problem; for $A > 4$ and NN plus 3N interactions, this matrix is sparse. The eigenvalues of this matrix are approximations to the energy levels, to be compared to the experimental binding energies and spectra, and the corresponding eigenvectors to the nuclear wave functions. Although the wave functions themselves are not observable, they can be employed to evaluate additional physical observables.

Conventionally, one uses a harmonic oscillator (HO) basis with energy parameter $\hbar \omega$ for the single-particle wave functions. A convenient and efficient truncation of the complete (infinite-dimensional) basis is a truncation on the total number of HO quanta: the basis is limited to many-body basis states with $\sum_A N_A \leq N_0 + N_{\text{max}}$, with $N_0$ the minimal number of quanta for that nucleus and $N_{\text{max}}$ the truncation parameter. (Even (odd) values of $N_{\text{max}}$ provide results for natural (unnatural) parity.) Numerical convergence toward the exact results for a given Hamiltonian is obtained with increasing $N_{\text{max}}$, and is marked by approximate $N_{\text{max}}$ and $\hbar \omega$ independence. In practice we use extrapolations to estimate the binding energy in the complete (but infinite-dimensional) space [2, 3, 4, 5, 6], based on a series of calculations in finite bases.

The rate of convergence depends both on the nucleus and on the interaction. For realistic interactions, the dimension of the matrix needed to reach a sufficient level of convergence is in the billions, and the number of nonzero matrix elements is in the tens of trillions, which saturates available storage on current computing facilities. All NCCI calculations presented here were performed on the Cray XC30 Edison and Cray XC40 Cori at NERSC and the IBM BG/Q Mira at Argonne National Laboratory, using the code MFDn [7, 8].

2. Nuclear Interactions from Chiral Effective Field Theory
Chiral Effective Field Theory ($\chi$EFT) allows us to derive nuclear interactions (and the corresponding electroweak current operators) in a systematic way [9, 10, 11]. The chiral expansion is by no means unique: e.g. different choices for the functional form of the regulator and/or different choices for the degrees of freedom lead to different $\chi$EFT interactions. With the LENPIC collaboration [12, 13, 14] we use the same $\chi$EFT interactions for ab initio calculations ranging from nucleon-nucleon and nucleon-deuteron scattering to the structure of medium-mass nuclei. Specifically, here we use the semilocal coordinate-space regularized chiral potentials of Refs. [15, 16] to calculate the binding energies and spectra of $p$-shell nuclei. The leading order (LO) and next-to-leading order (NLO) contributions are given by NN-only potentials while 3NFs appear first at next-to-next-to-leading order ($N^2$LO) in the chiral expansion [10, 11].

Four-nucleon forces are even more suppressed and start contributing at $N^3$LO. The chiral power counting thus provides a natural explanation of the observed hierarchy of nuclear forces. The Low-Energy Constants (LECs) in the NN-only potentials of Refs. [15, 16] have been fitted to nucleon-nucleon scattering, without any input from nuclei with $A > 2$. The 3NFs at $N^3$LO involve two LECs which govern the strength of the one-pion-exchange-contact term and purely contact 3NF contributions. Conventionally, these LECs are expressed in terms of two dimensionless parameters $c_D$ and $c_E$. Obviously, these LECs cannot be fixed from nucleon-nucleon scattering; they have to be fitted to select 3-body (or higher $A$-body) observables. We follow the commonly adopted practice [17, 18, 19, 20] and use the $^3$H binding energy as one of the observables; this gives us a correlation between $c_D$ and $c_E$.

A wide range of observables has been considered in the literature to constrain the remaining LEC. In Ref. [14] different ways to fix this LEC in the 3-nucleon sector were explored, and it was shown that it can be reliably determined from the minimum in the differential cross section in elastic nucleon-deuteron scattering at intermediate energies. This allows us to make parameter-free calculations for $A \geq 4$ nuclei. In these proceedings we present an overview of the ground
state energies for all stable $p$-shell nuclei (excluding mirror nuclei), as well as excitation spectra for selected nuclei up to $A = 12$, all obtained with the same semilocal regulator $R = 1.0$ fm and the same LECs. Specifically, the LECs values for the 3NFs at NLO are $c_D = 7.2$ and $c_E = -0.671$, as determined in Ref. [14]. Application of these interactions to nucleon-deuteron scattering can be found in Refs. [12, 13] for NN-only potentials, along with selected properties of light- and medium-mass nuclei, and in Ref. [14] including the 3NFs at N2LO.

3. Ground State Energies for $p$-shell Nuclei

Here we present our results for the ground state energies of the stable $p$-shell nuclei, excluding mirror nuclei, all obtained with the same semilocal chiral interactions up to N2LO. In Fig. 1 we show the ground state ($J^P = 1^+$) energy of $^6$Li as function of the HO basis parameter $\hbar\omega$ for a range of $N_{\text{max}}$ values. With NN-only potentials, we can perform calculations up to $N_{\text{max}} = 18$ for $A = 6$ nuclei. This is sufficient to achieve a reasonable level of convergence, as can be seen from the left three panels of Fig. 1. With 3NFs however, we are limited to significantly smaller bases, and in order to improve the numerical convergence with basis size we therefore first perform a Similarity Renormalization Group (SRG) transformation [21, 22, 23] on the Hamiltonian. The right-most panel of Fig. 1 shows results for the ground state energy of $^6$Li at N2LO including 3NFs at a very modest SRG flow parameter $\alpha = 0.02$ fm$^4$ (note that $\alpha = 0$ correspond to the original Hamiltonian, without SRG), for calculations up to $N_{\text{max}} = 12$. Indeed, the convergence with increasing $N_{\text{max}}$ is significantly improved with this SRG-evolved interaction compared to the bare NN-only interactions at NLO and N2LO. At $N_{\text{max}} = 12$ the level of convergence is already comparable to that of the bare NLO and N2LO potentials at $N_{\text{max}} = 16$. Also note that the variational minimum in $\hbar\omega$ shifts to lower values due to the SRG evolution.

In Fig. 2 we show the ground state energies of $^7$Li (left, $J^P = \frac{3}{2}^-$) and $^{10}$B (right, $J^P = 3^+$) as function of $N_{\text{max}}$ at fixed $\hbar\omega$ values close to the variational minimum with the N2LO interaction with and without explicit 3NFs. Based on these results in finite bases, we can use extrapolations to the complete (infinite-dimensional) basis. Here we use a three parameter fit at fixed $\hbar\omega$ at or just above the variational minimum

$$E(N_{\text{max}}) \approx E_{\infty} + a \exp (-b N_{\text{max}}),$$

Figure 1. (Color online) Calculated ground state energy of $^6$Li using chiral LO, NLO, and N2LO interactions at $R = 1.0$ fm as function of the basis HO parameter $\hbar\omega$ for $N_{\text{max}} = 2$ to 18 for NN-only potentials (left 3 panels) and at N2LO w. 3NFs, SRG-evolved to $\alpha = 0.02$ fm$^4$ for $N_{\text{max}} = 2$ to 12 (right-most panel). The dotted horizontal line is the experimental value.
which seems to work well for a range of interactions and nuclei [2, 24, 25]. The lines in Fig. 2 correspond to the extrapolating function fitted to the three highest available $N_{\text{max}}$ values.

Again, with the SRG-evolved interactions the ground state energies converge more rapidly with $N_{\text{max}}$ than with the bare (black dots and curves) NN-only N$^2$LO interaction. However, as a consequence of the SRG transformation, our results do depend on the SRG flow parameter $\alpha$, because we do not incorporate any induced interactions beyond 3NFs. Without explicit 3NFs, this dependence seems to be negligible, and typically less than the extrapolation uncertainty – the bare NN-only N$^2$LO interaction and the two SRG-evolved interaction with induced 3NFs extrapolate to approximately the same value. On the other hand, with explicit 3NFs there is a weak but noticeable dependence on the SRG parameter $\alpha$, as can be seen by the spread of the red extrapolation curves in Fig. 2. This $\alpha$ dependence is due to induced 4-body (and higher-body) interactions which we have neglected.

In Table 1 we summarize our results up to N$^2$LO for the ground state energies of stable $p$-shell nuclei, excluding mirror nuclei, extrapolated to the complete basis. Our estimate of the extrapolation uncertainty is based on the difference with smaller $N_{\text{max}}$ extrapolations, as well as the basis $\hbar \omega$ dependence over an 8 to 12 MeV span in $\hbar \omega$ values around the variational minimum, adjusted to be at least 20% of the difference with the variational minimum [13].

With NN-only potentials we use the bare interaction up to $A = 10$, for which we can perform calculation at $N_{\text{max}} = 12$ or higher. For select nuclei with $11 \leq A \leq 16$ we use the SRG-evolved interaction at $\alpha = 0.04$ fm$^4$ with induced 3NFs for NN-only potentials up to $N_{\text{max}} = 8$. At N$^2$LO with explicit 3NFs we present results with SRG-evolved interactions at both $\alpha = 0.04$ fm$^4$ and $\alpha = 0.08$ fm$^4$. As expected, the calculations at $\alpha = 0.08$ fm$^4$ are better converged, and have therefore a smaller extrapolation uncertainty than those at $\alpha = 0.04$ fm$^4$. The anticipated $\alpha$ dependence appears to be of the same order of magnitude as the extrapolation uncertainty.

Generally, the agreement with the experimental binding energies improves as one goes from LO to NLO to N$^2$LO. At LO all $p$-shell nuclei are significantly overbound, but at N$^2$LO the binding energies of nuclei up to $A = 12$ are within few percent of the experimental values. As $A$ increases beyond $A = 12$, the nuclei become more and more overbound – $^{12}\text{C}$ is overbound by about 3% whereas $^{16}\text{O}$ is overbound by about 13%. The overbinding of $^{16}\text{O}$ is significantly larger than the estimated chiral truncation uncertainty [13], even with the inclusion of the explicit 3NFs [14], and it is as of yet unclear what the origin of this overbinding is.

At NLO and higher, we obtain the correct spin and parity for the ground states of most $p$-shell

Figure 2. (Color online) Calculated ground state energies using chiral N$^2$LO interactions at $R = 1.0$ fm as function of $N_{\text{max}}$ at the variational minimum in $\hbar \omega$ for $^7\text{Li}$ (left) and $^{10}\text{B}$ (right). The dotted horizontal line is the experimental value.
Table 1. Ground state energies of stable $A = 4$ to 16 nuclei with $\chi$EFT interactions up to N$^2$LO using $R = 1.0$ fm [13, 14]. The uncertainty estimate is only the extrapolation uncertainty in the many-body calculation, and does not include the chiral truncation error, nor uncertainties in the LECs. Entries with an asterisk * indicate excited states for nuclei where the calculated and experimental ground states have different $J^P$. Experimental values are extracted from Ref. [26].

| Nucleus | $J^P$ | LO NN-only | NLO NN-only | N$^2$LO NN-only | N$^2$LO including 3NFs $\alpha = 0.04$ fm$^4$ | N$^2$LO including 3NFs $\alpha = 0.08$ fm$^4$ | expt. |
|---------|------|------------|-------------|----------------|---------------------------------|---------------------------------|------|
| $^4$He 0$^+$ | $-$45.453(6) | $-$28.53(4) | $-$28.11(1) | $-$28.202(5) | $-$28.298(2) | $-$28.296 |
| $^6$He 0$^+$ | $-$43.2(2) | $-$28.7(2) | $-$27.9(2) | $-$28.55(15) | $-$28.79(8) | $-$29.27 |
| $^6$Li 1$^+$ | $-$46.7(1) | $-$31.6(2) | $-$31.0(2) | $-$31.49(16) | $-$31.72(6) | $-$31.99 |
| $^7$Li 3$^-$ | $-$57.1(2)* | $-$38.7(3) | $-$38.0(4) | $-$38.72(16) | $-$38.99(6) | $-$39.24 |
| $^8$He 0$^+$ | $-$39.8(6) | $-$29.7(5) | $-$27.8(6) | $-$29.5(3) | $-$29.9(2) | $-$31.41 |
| $^8$Li 2$^+$ | $-$55.7(5) | $-$40.3(7) | $-$39.0(8) | $-$40.4(4) | $-$40.7(2) | $-$41.28 |
| $^9$Li 0$^+$ | $-$87.7(4) | $-$56.0(7) | $-$55.4(9) | $-$55.6(5) | $-$56.1(3) | $-$56.50 |
| $^9$Be 2$^-$ | $-$57.1(4) | $-$43.9(7) | $-$41.7(8) | $-$43.9(4) | $-$44.0(2) | $-$45.34 |
| $^{10}$Be 2$^-$ | $-$84.7(7) | $-$58.0(1.4) | $-$56.4(1.5) | $-$57.5(5) | $-$58.0(3) | $-$58.16 |
| $^{11}$Be 0$^+$ | $-$92.2(8) | $-$65.2(1.5) | $-$62.8(1.7) | $-$64.1(9) | $-$64.5(9) | $-$64.98 |
| $^{10}$B 3$^+$ | $-$88.1(1.2)* | $-$64.6(1.5)* | $-$63.2(1.7)* | $-$64.3(8) | $-$64.9(5) | $-$64.75 |
| $^{10}$B 1$^+$ | $-$93.9(8) | $-$64.9(1.8) | $-$63.1(1.9) | $-$63.1(1.0)* | $-$64.1(8)* | $-$64.03* |
| $^{11}$Be 1$^+$ | $-$108.1(1) | $-$76.8(6) | $-$73.9(7) | $-$77.2(9) | $-$77.7(5) | $-$76.21 |
| $^{11}$Be 2$^-$ | $-$89.5(1.4) | $-$69.8(9) | $-$69.8(9) | $-$69.8(9) | $-$69.8(9) | $-$69.8(9) |
| $^{12}$B 1$^+$ | $-$111.1(1.)* | $-$82.6(8) | $-$78.6(8) | $-$81.9(9)* | $-$82.5(5)* | $-$79.58 |
| $^{12}$B 2$^+$ | $-$111.1(1.)* | $-$82.3(9)* | $-$77.8(7)* | $-$82.9(8)* | $-$83.2(5) | $-$78.63* |
| $^{13}$C 0$^+$ | $-$139.1(1) | $-$95.5(7) | $-$92.7(6) | $-$94.7(1.0) | $-$95.5(5) | $-$92.16 |
| $^{13}$B 3$^-$ | $-$104.1(7.0) | $-$104.4(4) | $-$104.7(1.0) | $-$104.7(1.0) | $-$104.7(1.0) | $-$104.7(1.0) |
| $^{13}$C 5$^+$ | $-$116.0(1.3) | $-$116.1(5) | $-$116.1(5) | $-$116.1(5) | $-$116.1(5) | $-$116.1(5) |
| $^{14}$N 1$^+$ | $-$117.3(1.3) | $-$117.4(4) | $-$117.4(4) | $-$117.4(4) | $-$117.4(4) | $-$117.4(4) |
| $^{15}$N 0$^+$ | $-$130.4(1.6) | $-$131.0(6) | $-$131.0(6) | $-$131.0(6) | $-$131.0(6) | $-$131.0(6) |
| $^{16}$O 0$^+$ | $-$223.2(4) | $-$152.1(1) | $-$146.1(1) | $-$144.2(2) | $-$145.2(8) | $-$127.62 |

nuclei – the exceptions are $^{10}$B, $^{11}$Be, and $^{12}$B, for which we include both the experimental and the calculate ground states in Table 1. For $^{10}$B, the NN-only interactions produce a $J^P = 1^+$ ground state, whereas the experimental ground state has $J^P = 3^+$. With the consistent explicit 3NFs at N$^2$LO we are able to reproduce the experimental ground state for $^{10}$B, in agreement with previous studies of $^{10}$B with $\chi$EFT interactions [19, 25]. For $^{12}$B the situation is the opposite: at NLO and N$^2$LO without the 3NFs we do find the correct ground state, $J^P = 1^+$, but adding the 3NFs to the N$^2$LO NN potential leads to a ground state with $J^P = 2^+$, and the $J^P = 1^+$ state becomes the first excited state, with an excitation energy of about 1 MeV. It remains to be seen whether or not this discrepancy gets resolved at higher order in the chiral expansion.
The situation in $^{11}\text{Be}$ is different: here we have a nucleus with parity inversion, that is, the ground state has the opposite parity of what one would expect based on the shell-model. In NCCI calculations the ‘natural’ and ‘unnatural’ parity states are expressed in bases with even or odd $N_{\text{max}}$ values respectively. For $^{11}\text{Be}$ that means the negative parity states are calculated in bases with even $N_{\text{max}}$ and the positive parity states states in bases with odd $N_{\text{max}}$. We then perform an extrapolation to the complete basis for the lowest state with even $N_{\text{max}}$ as well as for the lowest state with odd $N_{\text{max}}$. This leads to the energies listed in Table 1 for the $\frac{1}{2}^+$ state (the experimental ground state) and for the the $\frac{1}{2}^-$ state (the lowest natural parity state). Although the latter has a lower energy in our calculations, the difference with that of the $\frac{1}{2}^+$ is less than the extrapolation uncertainty, and within their uncertainties, both energies agree with the experimental values. In order to reliably determine which of these two states is the ground state we should use more sophisticated calculational methods for this system and follow e.g. the approach discussed in Ref. [27] for $^{11}\text{Be}$.

4. Excitation Spectra for $p$-shell Nuclei
In addition to the ground state energies, we also obtain the energy levels of excited states. The energy differences with the ground state generally converge significantly better than the actually binding energies of excited states, at least for states of the same parity. In Fig. 3 we show the low-lying spectra of $^6\text{Li}$ and $^7\text{Li}$ as function of the HO basis parameter $h\omega$ for several of $N_{\text{max}}$ values. Again, with NN-only potentials we achieve a reasonable level of convergence, in particular for narrow excited states like the $3^+$ state in $^6\text{Li}$ and the $\frac{1}{2}^-$ and $\frac{7}{2}^-$ states in $^7\text{Li}$. The persistent increase of the excitation energies of with increasing $h\omega$ for the higher excited states suggest that these are (significantly) broader, and therefore poorly converging in a HO basis. Indeed, the two $2^+$ states in $^6\text{Li}$ are broad; and although the $0^+$ in $^6\text{Li}$ (the analog state of $^6\text{He}$) is narrow, in our calculations with NN-only interactions up to N$^2$LO, $^6\text{He}$ is not or barely bound, see Table 1; hence, with these interactions this state will be broad and poorly converging.

At LO the spectra do not agree with experiment – most excitation energies are too large, and often the order of the states is incorrect: e.g. in $^7\text{Li}$ the ground state, $\frac{3}{2}^-$, and the first excited state, $\frac{1}{2}^-$, are essentially degenerate. Indeed, the LO potential is not very realistic – not only is it significantly too attractive (it overbinds all $p$-shell nuclei by up to a factor of two), it is also missing e.g. essential spin-orbit couplings. However, starting at NLO the spectra tend to be in qualitative agreement with data. At N$^2$LO with explicit 3NFs we use SRG evolution to improve convergence of the NCCI calculations. The dependence of the excitation energies on the SRG parameter $\alpha$ is negligible, much smaller than the $h\omega$ dependence, as can be seen in the the right-most panels of Fig. 3. Generally, inclusion of the 3NFs improves agreement with experiment (see also Fig. 9 of Ref. [14]). In particular, we see in Fig. 3 that the excitation energy of the $3^+$ state of $^6\text{Li}$ moves slightly closer to experiment; and in $^7\text{Li}$ the $\frac{7}{2}^-$ also moves slightly closer to experiment. Furthermore the second $\frac{5}{2}^-$ state becomes much better converged while the first $\frac{5}{2}^-$ exhibits a persistent $h\omega$ dependence, suggesting that the first $\frac{5}{2}^-$ is broad, and the second narrow, both in agreement with data.

In Fig. 4 we show the low-lying positive-parity spectra for $^8\text{Li}$, $^8\text{Be}$, and $^{10}\text{Be}$ at N$^3$LO with explicit 3NFs, SRG evolved to $\alpha = 0.04$ fm$^{-1}$ (solid) and 0.08 fm$^{-1}$ (dashed). Again, the SRG dependence is negligible compared to the $h\omega$ dependence, except for the high-lying pairs of $2^+$, $1^+$, and $3^+$ in $^8\text{Be}$; given this SRG dependence, the spectrum of $^8\text{Be}$ is in quite reasonable agreement with the data. For $^8\text{Li}$ we do find the known narrow $1^+$, $3^+$, and $4^+$ states, as well as two poorly converged (i.e. broad) $1^+$ states, all in reasonabe agreement with experiment; in addition we find one $0^+$ state, as well as two $2^+$ states, all poorly converged.

The first excited state in $^{10}\text{Be}$, with $J^P = 2^+$, is quite well converged, and in excellent
agreement with the experimental excitation energy. We also do find two additional $2^+$ states among the lowest five states in qualitative agreement with data, but not as well converged. However, we do not find any low-lying $0^+$ state in our calculations, in contrast to experiment; we will come back to this when discussing $^{12}$C below. Furthermore, our calculations suggest that there is a $1^+$ state between the second and third $2^+$ excited state.

The low-lying spectra for $^{10}$B up to $N^{2LO}$ are shown in Fig. 5; in addition to the ground state $3^+$, two low-lying $1^+$ states, and a low-lying $2^+$, there is also the $0^+$ analog state of the ground state of $^{10}$Be which is not shown. At LO the calculated spectrum does not look like the experimental spectrum at all: the lowest state is a $1^+$ state, followed by three nearly degenerate states, with $J^P = 2^+$, $3^+$, and $1^+$, respectively, at excitation energies of about 6 MeV. At NLO and NN-only $N^{2LO}$ the agreement with experiment is noticeably better, except for the ordering of the $3^+$ ground state and the lowest $1^+$ state. This is a known issue, and the general consensus
is that 3NFs are needed to achieve the proper $3^+$ ground state for $^{10}\text{B}$ [19, 25]. Indeed, adding the 3NFs at N$^2$LO does give the correct ground state, followed by two $1^+$ states with excitation energies of a few MeV. However, these two low-lying $1^+$ states mix, with the amount of mixing strongly dependent on the basis $\hbar \omega$ and $N_{\text{max}}$ parameters, which makes it difficult to extract actual excitation energies for these two states [25]. The lowest $2^+$ is in reasonable agreement with the data at N$^2$LO with 3NFs.

Figure 4. (Color online) Positive-parity excitation spectra of $^{8}\text{Li}$, $^{8}\text{Be}$, and $^{10}\text{Be}$ using the chiral N$^2$LO interaction w. 3NFs, SRG-evolved to $\alpha = 0.04$ fm$^4$ (solid) and $\alpha = 0.08$ fm$^4$ (dashed), as function of the basis HO parameter $\hbar \omega$, with $N_{\text{max}} = 10$ for $^{8}\text{Li}$ and $^{8}\text{Be}$ and $N_{\text{max}} = 8$ for $^{10}\text{Be}$. Experimental levels from ENSDF, Ref. [29].

Figure 5. (Color online) Calculated positive-parity excitation spectrum of $^{10}\text{B}$ using chiral LO, NLO, and N$^2$LO interactions at $R = 1.0$ fm as function of the basis HO parameter at $N_{\text{max}} = 8$ for NN-only potentials (left 3 panels) and for N$^2$LO w. 3NFs (right-most panel), all SRG-evolved to $\alpha = 0.04$ fm$^4$ (solid) and $\alpha = 0.08$ fm$^4$ (dashed). Note the different vertical offset for the LO panel. The dotted horizontal lines are the experimental values [29].
Finally, in Fig. 6 we show the low-lying positive-parity spectra for $^{12}$B and $^{12}$C. Again, at LO the spectra do not agree with experiment; furthermore, we do not find the Hoyle state in $^{12}$C (nor any of its rotational excitations) due to the known limitations of the HO basis [31]. Furthermore, our spectra at NLO and N$^2$LO show a significant sensitivity to the chiral order, as well as the 3NFs at N$^2$LO, for both of these two nuclei.

In particular, at N$^2$LO with 3NFs the first excited $2^+$ state in $^{12}$B becomes the ground state in our calculations, and the splitting between this state and the other excited states is significantly too large. On the other hand, the energy differences of the $0^+$, the second $2^+$, the $1^+$, and the $3^+$ relative to the lowest $1^+$ state are in better agreement with 3NFs than without 3NFs at N$^2$LO. Possibly even more puzzling, though not surprising, is the lowest $1^+$ excited state in $^{12}$C [32]. At NLO it is in reasonable agreement with experiment, just below the $4^+$ rotational excitation of the ground state; at N$^2$LO without 3NFs, the order of the $1^+$ and the $4^+$ is reversed; and

![Graphical representation of spectra](image)

**Figure 6.** (Color online) Calculated positive-parity excitation spectrum of $^{12}$B (top) and $^{12}$C (bottom) using chiral LO, NLO, and N$^2$LO interactions at $R = 1.0$ fm as function of the basis HO parameter at $N_{\text{max}} = 8$ for NN-only potentials (left 3 panels) and for N$^2$LO w. 3NFs (right-most panel), all SRG-evolved to $\alpha = 0.04$ fm$^4$ (solid) and $\alpha = 0.08$ fm$^4$ (dashed). The dotted horizontal lines are the experimental values [30].
including the 3NFs at N^2LO reduces the excitation energy of the 1^+ by about 5 MeV, destroying the qualitative agreement with experiment. Note that this shift due to the 3NFs is significantly larger than that for the 2^+ state in ^{12}\text{B}, which is of the order of 2 MeV.

In conclusion most spectra for p-shell nuclei up to to \( A = 12 \), calculated at N^2LO with 3NFs, agree reasonably well with the experimental data, in particular for narrow states. The exceptions are two states, in ^{12}\text{B} and ^{12}\text{C} respectively. The low-lying spectra of ^{10}\text{B} and ^{12}\text{B}, together with the excitation energy of the lowest 1^+ state in ^{12}\text{C}, could play a critical role in determining accurate NN and 3N interactions for the upper p-shell and beyond. Indeed, both the 2^+ state in ^{12}\text{B} and the 1^+ state in ^{12}\text{C} are sensitive to e.g. the LECs \( c_D \) and \( c_E \).

Acknowledgments
This work was supported by the US Department of Energy under Grant No. DE-SC0018223 (SciDAC-4/NUCLEI) and the Fundação de Amparo à Pesquisa do Estado de São Paulo, Brazil (FAPESP) under Grant No. 2017/19371-0. This research used resources of the National Energy Research Scientific Computing Center (NERSC) and the Argonne Leadership Computing Facility (ALCF), which are US Department of Energy Office of Science user facilities, supported under Contracts No. DE-AC02-05CH11231 and No. DE-AC02-06CH11357, and computing resources provided under the INCITE award ‘Nuclear Structure and Nuclear Reactions’ from the US Department of Energy, Office of Advanced Scientific Computing Research.

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