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Ab initio nuclear structure simulations: The speculative ^{14}F nucleus

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We present results from *ab initio* no-core full configuration simulations of the exotic proton-rich nucleus ^{14}F, whose first experimental observation is expected soon. Calculations with the JISP16 NN interaction are performed up to the $N_{\max} = 8$ basis space. The binding energy is evaluated using an extrapolation technique. This technique is generalized to excitation energies, verified in calculations of ^{6}Li, and applied to ^{14}F and ^{14}B, the ^{14}F mirror, for which some data are available.

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Exotic nuclei at the nucleon drip lines and beyond constitute a forefront research area in nuclear physics. The physics drivers include (1) discovering how shell structures evolve into extreme isospin regions and (2) extending our knowledge of strong interactions, especially elusive three-nucleon forces (3NFs), under these conditions. To help pave a path toward these goals, we present baseline *ab initio* results for selected unstable $A = 13$ and $A = 14$ nuclei.

We focus especially on ^{14}F, with isospin $T = 2$, which is expected to lie beyond the proton drip line and therefore be unstable. This proton-rich nucleus will strain the convergence properties of the *ab initio* methods we adopt here and, also, push the limits of state-of-the-art experimental facilities. Indeed, the first experimental results regarding this four-proton-excess isotope will be available soon from the Cyclotron Institute at Texas A&M University [1].

We perform the first *ab initio* study of ^{14}F. We use the no-core shell model (NCSM) [2,3], which employs a many-body harmonic oscillator basis that treats all nucleons as spectroscopically active. The basis space includes all many-body states with excitation quanta less than or equal to $N_{\max}$, which makes it possible to completely remove spurious center-of-mass excitations. We used the code MFDn [4–6] and the realistic NN interaction JISP16[1] [7], which is known to provide a good description of p-shell nuclei [7,8] without an additional 3NF. The largest calculations were performed in the $N_{\max} = 8$ basis space, which for this nucleus contains 1 990 061 078 basis states with total magnetic projection $M = 0$ and natural parity (negative). Determination of the lowest 10 to 15 eigenstates of the sparse Hamiltonian matrix, for each oscillator parameter $\hbar\Omega$, requires 2 to 3 h on 7 626 quad-core compute nodes at the Jaguar supercomputer at Oak Ridge National Laboratory.

We show our complete results for the ^{14}F ground-state energy in Fig. 1. The solid curves are our NCSM results with the bare interaction JISP16. These results are strict upper bounds for the ground-state energy and converge monotonically with $N_{\max}$ to the infinite basis space results. The dashed curves in Fig. 1 were obtained in more conventional NCSM calculations with effective NN interactions derived from the initial bare interaction JISP16 by the Lee-Suzuki-Okamoto (LSO) renormalization procedure [9]. The renormalization procedure is truncated at the two-body cluster level—that is, induced three-body, four-body, etc., contributions are neglected; hence we refer to these calculations as LSO(2) renormalized. Note that these results differ slightly from preliminary approximate results presented at recent conferences [10,11].

Comparing the bare and LSO(2) renormalized JISP16 results in Fig. 1, we observe that the tendency of the LSO(2) renormalized calculations is misleading. For increasing basis spaces from $N_{\max} = 0$ to 6, the minimum of the $\hbar\Omega$-dependent curves increases, suggesting an approach from below to the infinite basis space result. At $N_{\max} = 6$, the LSO(2) renormalized JISP16 produces a nearly flat region at approximately the same energy as the minimum obtained with the bare JISP16 interaction. On the other hand, the bare interaction provides a variational upper bound for the ground-state energy, which decreases with increasing $N_{\max}$.

Other light nuclei (^{6}He, ^{6}Li, ^{8}Be, ^{12}C, ^{16}O, etc.) show a qualitatively similar behavior: the LSO renormalized interactions produce results that are neither an upper bound nor a lower bound, and the approach to the infinite basis space is nonmonotonic. Hence the convergence pattern of the LSO renormalized results is difficult to assess. Furthermore, with the patterns displayed in Fig. 1 for JISP16, the minima of the $\hbar\Omega$-dependent ground-state energy curves for both the bare and the LSO(2) renormalized interaction may be expected to coincide for $N_{\max} \geqslant 8$ as in some other nuclei. For these reasons, we did not perform expensive $N_{\max} = 8$ LSO(2) renormalized JISP16 calculations for ^{14}F.

Recently we introduced the *ab initio* no-core full configuration (NCFC) approach [8,12], by extrapolating NCSM results with the bare interaction in successive basis spaces to the infinite basis space limit. This makes it possible to obtain basis-space-independent results for binding energies and to evaluate their numerical uncertainties. We use two extrapolation methods: a global extrapolation, based on the calculations in four successive basis spaces and five $\hbar\Omega$ values in a 10-MeV interval (extrapolation A); and extrapolation B, based on the calculations at various fixed $\hbar\Omega$ values in three successive basis spaces and defining the most reliable $\hbar\Omega$ value for the

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[1]A Fortran code for the JISP16 interaction matrix elements is available at http://nuclear.physics.iastate.edu.

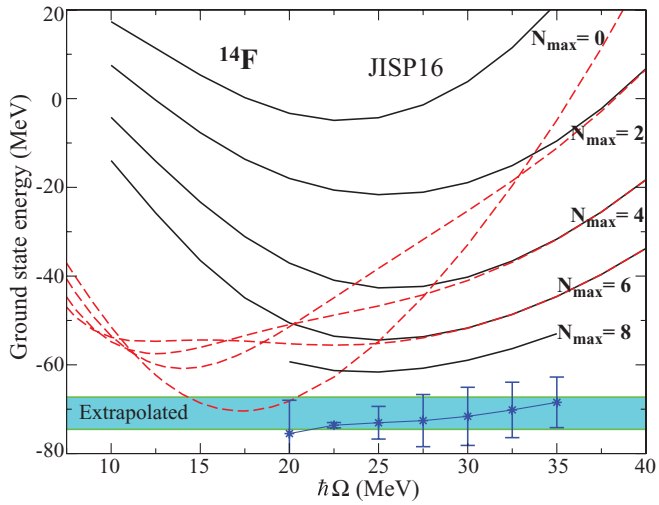

FIG. 1. (Color online) Results for the ground-state energy of ^{14}F with bare (solid lines) and LSO(2) renormalized (dashed lines) JISP16 as a function of the oscillator parameter $\hbar\Omega$. The shaded area demonstrates global extrapolation A for the binding energy and its uncertainty; extrapolation B at fixed $\hbar\Omega$ is given by asterisks. The most reliable $\hbar\Omega$ value for this extrapolation method is at $\hbar\Omega =$ 25 MeV for ^{14}F, with its uncertainty indicated by the error bar.

extrapolation. These extrapolations provide consistent results [8]. Combining both extrapolation methods suggests a binding energy of 72 ± 4 MeV for ^{14}F, which agrees well with AME03 nuclear binding energy extrapolations [14]; see Table I. Ironically, of all our NCSM calculations, with both the bare and the LSO(2) renormalized interaction, the minimum of the LSO(2) calculations at $N_{max} = 0$ appears to be closest to the infinite basis space result.

To check the accuracy of our approach, we performed similar calculations for the mirror nucleus ^{14}B, with a known binding energy of 85.423 MeV [13]. This value agrees with our NCFC result of 86 ± 4 MeV. We also performed NCFC calculations of the neighboring nucleus ^{13}O using basis spaces up to $N_{max} = 8$. The calculated binding energy of 77 ± 3 MeV also agrees with the experimental value of 75.556 MeV [13].

We note that a good description of both ^{14}F and ^{13}O in the same approach is important to have a consistent description of the $^{13}\mathrm{O} + p$ reaction that produces ^{14}F. In this way, any experimentally observed resonances can be directly compared with the difference in our results for the ^{14}F and ^{13}O energies. In this respect it is interesting to note that although the total energies of extrapolations A and B differ by about 2 MeV, the differences among the ground-state energies of these three nuclei are almost independent of the extrapolation method: for ^{14}F and ^{13}O the predicted difference is 4.6 MeV, and for ^{14}F and ^{14}B it is 13.5 MeV. (The numerical uncertainty in these differences is unclear but expected to be significantly smaller than the uncertainty in the total energies.)

TABLE I. NCFC results obtained with JISP16 for ground-state energies (MeV) of ^{13}O, ^{14}B, and ^{14}F. Experimental data are taken from Ref. [13].

Nucleus	Extrapol. A	Extrapol. B	Experiment
^{13}O	−75.7(2.2)	−77.6(3.0)	−75.56(0.01)
^{14}B	−84.4(3.2)	−86.6(3.8)	−85.42(0.02)
^{14}F	−70.9(3.6)	−73.1(3.7)	−73.3(0.4)[a]

[a]AME03 extrapolation [14].

We also calculated the ^{14}F excitation spectrum in anticipation of the experimental results. It is unclear how to extrapolate excitation energies obtained in finite basis spaces, but we can extrapolate the total energies of excited states using the same methods as discussed previously for the ground-state energy. For the lowest state in each J^π channel the convergence pattern should be similar to that of the ground state; for excited states with the same quantum numbers we simply assume the same convergence pattern. We perform independent separate extrapolation fits for all states. The differences between the extrapolated total energies and the ground-state energy is our prediction for the excitation energies.

This approach to extrapolating the total eigenenergies is supported by applying it to ^{6}Li; see Table II. We have results for ^{6}Li in basis spaces up to $N_{max} = 16$, where a good convergence is achieved and hence the extrapolation uncertainties are small. These results are compared in Table II with the extrapolations based on calculations in basis spaces up to $N_{max} = 8$, that is, in the same basis spaces used for the ^{14}F and ^{14}B studies.

We see that the excitation energies based on $N_{max} = 8$ and smaller basis space results are consistent with the results obtained in larger spaces. The level ordering is the same and the difference between the $N_{max} = 8$ and the $N_{max} = 16$ results is generally much smaller than the estimated uncertainties in the total energies of the $N_{max} = 8$ extrapolations. This suggests that the numerical uncertainty in the excitation energies is significantly smaller than the uncertainty in the total energies: apparently, the calculated total energies share a significant systematic uncertainty, an overall binding uncertainty, which cancels when results are expressed as excitation energies. Furthermore, we see that both extrapolation methods agree very well with each other (within their error estimates) and that the error estimates decrease as one increases the basis space.

Extrapolation B leads to results for the two lowest excited states, which are practically independent of the oscillator parameter $\hbar\Omega$; see Fig. 2. Also, the bare and LSO renormalized NCSM results for these two states show very little dependence on $\hbar\Omega$. These states are narrow resonances and agree very well with experiment.

On the other hand, the three higher excited states have a much larger width; see Table II. Our calculations for these broad resonances show a significant dependence on both $\hbar\Omega$ and N_{max}, in particular, for the excited $(1^+, 0)_2$ state, which has the largest width. Extrapolation B to infinite model space reduces but does not eliminate the $\hbar\Omega$ dependence. We further note that the $\hbar\Omega$ dependence of these excitation energies is typical for wide resonances, as observed in comparisons of NCSM results with inverse scattering analysis of α-nucleon scattering states [16], and that the slope of the $\hbar\Omega$ dependence increases with the width of the resonance. This is consistent with the results presented in Fig. 2: the width of the $(1^+, 0)_2$ state is larger than the width of the $(2^+, 0)_2$ state; the latter

TABLE II. NCFC results for ^{6}Li ground-state E_{gs} and excitation E_x energies (MeV) obtained in different basis spaces with JISP16. For extrapolations A and B an estimate of the accuracy of the total energies is given in parentheses; for the LSO(2) renormalized interaction, the spread in excitation energy for $\hbar\Omega$ variations from 12.5 to 22.5 MeV is listed. Experimental data are taken from Ref. [15].

$E(J^\pi, T)$	Extrapol. A ($N_{max} = 2-8$)	Extrapol. ($N_{max} = 4-8$)	LSO(2) ($N_{max} = 6$)	Extrapol. A ($N_{max} = 10-16$)	Extrapol. B ($N_{max} = 12-16$)	LSO(2) ($N_{max} = 14$)	Experiment Energy	Experiment Width
$E_{gs}(1^+, 0)_1$	−30.9(0.6)	−31.1(0.3)		−31.47(0.09)	−31.48(0.03)		−31.994	Stable
$E_x(3^+, 0)$	2.6(0.5)	2.5(1.2)	2.2–2.7	2.56(0.04)	2.55(0.07)	2.53–2.55	2.186	24×10^{-3}
$E_x(0^+, 1)$	3.6(0.6)	3.5(1.2)	3.3–3.7	3.68(0.06)	3.65(0.06)	3.6–3.8	3.563	8.2×10^{-6}
$E_x(2^+, 0)$	5.3(0.9)	5.5(1.8)	4.8–5.8	4.5(0.1)	4.5(0.2)	4.8 − 5.0	4.312	1.30
$E_x(2^+, 1)$	6.3(0.7)	6.1(1.6)	6.2–6.5	5.9(0.1)	5.9(0.1)	6.0–6.4	5.366	0.54
$E_x(1^+, 0)_2$	6.1(1.7)	6.6(0.3)	7.1–8.5	5.4(0.3)	5.4(0.2)	6.1–6.6	5.65	1.5

is larger than the width of the $(2^+, 1)$ state. Thus, there appears to be a significant correlation between the resonance width and the $\hbar\Omega$ dependence. The validity of the extrapolation to infinite model space is not entirely clear for these states.

We noted earlier that the LSO renormalized interaction does not provide a monotonic approach to the infinite basis space for the binding energies and this prevents simple extrapolation. On the other hand, the excitation energies with the LSO renormalized interaction are often quite stable with N_{max}. However, it is important to realize that this does not necessarily mean that these excitation energies are numerically converged: they do depend on $\hbar\Omega$. The dependence of the excitation energies on $\hbar\Omega$ decreases slowly with increasing N_{max}, as reported in Table II. In fact, the excitation energies obtained with LSO(2) renormalized JISP16 are nearly the same as those obtained with the bare interaction, except at small values of $\hbar\Omega$, as illustrated in Fig. 2. For most states, the NCFC provides better results for the excitation energies, with less basis space dependence than the LSO(2) NCSM calculations in finite basis spaces. Nevertheless, we can employ the LSO procedure to obtain estimates of the binding and excitation energies in small basis spaces where there are no NCFC results.

We summarize our results for the spectra of ^{14}F and ^{14}B in Table III. The excitation energies are obtained as a difference between the extrapolated total energies of the excited state and that of the ground state (see Table I). The spectra are rather dense and the spacing between energy levels is smaller than the quoted numerical uncertainty, which is that of the extrapolated total energies of the excited states. However, as discussed above, we expect that for narrow resonances the actual numerical error in the excitation energy is (significantly) smaller than the error in the total energy.

Figure 3 shows that different excited states can have very different convergence behavior. (Although we present the ^{14}B results in Fig. 3, the behavior of the ^{14}F states is similar.) At $N_{max} = 8$, there are five low-lying excited states; the excitation energy of these states depends only weakly on the basis space as N_{max} increases from 2 to 8. Then there are numerous higher excited states that depend strongly on the basis space: their excitation energies decrease rapidly with increasing N_{max}. Only after extrapolation to the infinite basis space do they

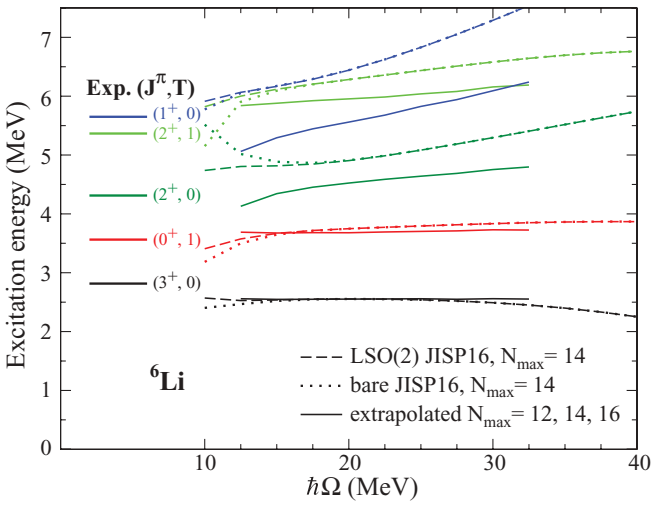

FIG. 2. (Color online) NCSM results for the spectrum of ^{6}Li with LSO(2) renormalized (dashed lines) and bare (dotted lines) JISP16 at $N_{max} = 14$, compared to NCFC extrapolations to infinite basis space (solid lines). Experimental (exp.) data are from Ref. [15].

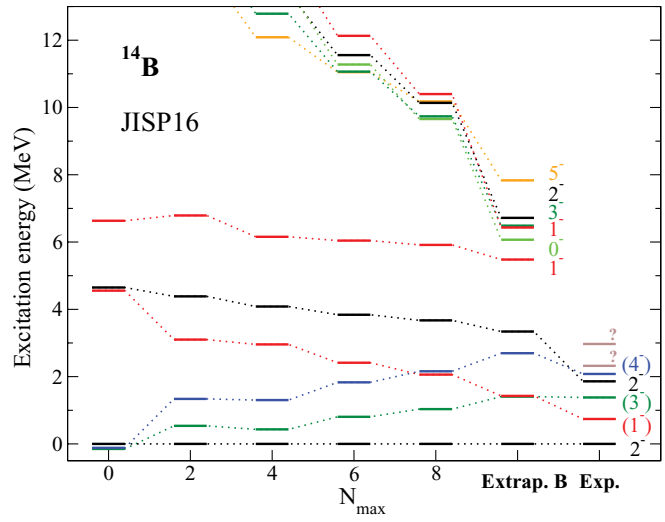

FIG. 3. (Color online) Negative-parity ^{14}B spectrum obtained with JISP16 at fixed $\hbar\Omega = 25$ MeV in successive basis spaces and extrapolated to infinite basis space using extrapolation B. Experimental (exp.) data are taken from Ref. [13].

TABLE III. NCFC results for ^{14}F and ^{14}B excitation energies E_x (MeV). For extrapolations A and B an estimate of the accuracy of the total energies is given in parentheses; for the LSO(2) renormalized interaction, the spread in excitation energy for $\hbar\Omega$ variations from 12.5 to 22.5 MeV is listed. Experimental data are taken from Ref. [17].

$E(J^\pi, T)$	NCFC and NCSM *ab initio* calculations with JISP16						Experiment:	
	^{14}F			^{14}B			^{14}B	
	Extrap. A	Extrap. B	LSO(2) ($N_{max} = 6$)	Extrap. A	Extrap. B	LSO(2) ($N_{max} = 6$)	J^π	Energy
$E_x(1^-, 2)_1$	0.9(3.9)	1.3(2.5)	1.4–2.2	1.1(3.5)	1.4(2.8)	1.4–2.3	(1^-)	0.654(0.009)[a]
$E_x(3^-, 2)_1$	1.9(3.3)	1.5(4.6)	1.0–1.8	1.7(2.9)	1.4(4.6)	1.0–2.1	(3^-)	1.38(0.03)
$E_x(2^-, 2)_2$	3.2(3.5)	3.3(3.5)	3.3–3.7	3.3(3.1)	3.3(3.8)	3.5–3.8	2^-	1.86(0.07)
$E_x(4^-, 2)_1$	3.2(3.2)	2.8(4.8)	2.0–2.6	3.1(2.9)	2.7(4.8)	2.0–3.1	(4^-)	2.08(0.05)
							?	[2.32(0.04)][b]
							?	2.97(0.04)
$E_x(1^-, 2)_2$	5.9(3.5)	5.4(4.6)	5.8–6.4	5.9(3.1)	5.5(4.8)	5.7–6.4		
$E_x(0^-, 2)$	5.1(5.4)	5.8(1.0)	5.8–10.5	5.5(4.8)	6.1(1.4)	4.9–10.4		
$E_x(1^-, 2)_3$	6.2(4.8)	6.3(2.8)	7.2–11.5	6.4(4.3)	6.4(3.1)	6.1–11.3		
$E_x(2^-, 2)_3$	6.4(4.6)	6.3(3.4)	7.3–10.9	6.9(4.1)	6.7(3.6)	6.6–10.9		
$E_x(3^-, 2)_2$	6.9(4.2)	6.4(4.6)	7.6–10.6	7.0(3.7)	6.5(4.7)	6.4–10.5		
$E_x(5^-, 2)$	8.9(3.5)	7.9(5.9)	9.2–11.0	8.8(3.1)	7.8(5.9)	8.5–10.8		

[a]Updated from Ref. [18].

[b]The existence of this state is uncertain (see Ref. [17]).

appear at excitation energies comparable to those of the other low-lying excited states. We see a similar phenomenon in NCFC calculations of other nuclei.

The dependence on $\hbar\Omega$ varies considerably over the excited states as shown in Fig. 4. The lowest five excited states have a weak dependence on $\hbar\Omega$, whereas the higher excited states depend strongly on it. We expect our results for these higher excited states to have a larger numerical error than our results for the lower excited states with the weaker $\hbar\Omega$ dependence. Furthermore, in analogy to the excited states in ^{6}Li discussed above, we expect these higher states to be broad

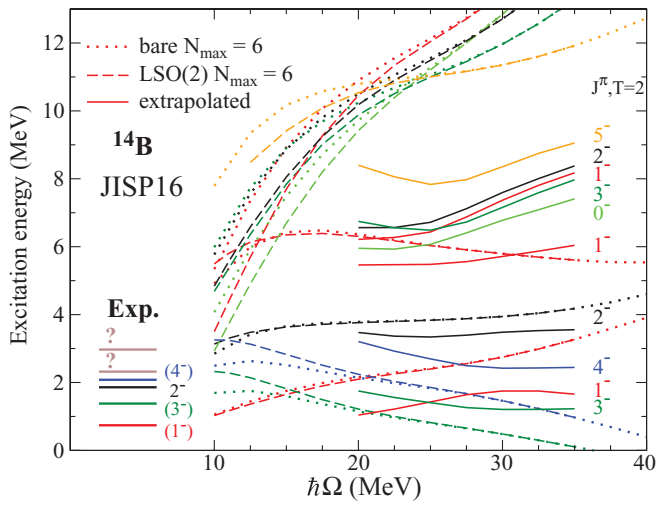

FIG. 4. (Color online) NCSM results for the negative-parity spectrum of ^{14}B with LSO(2) renormalized (dashed lines) and bare (dotted lines) JISP16 at $N_{max} = 6$, compared to NCFC extrapolations to infinite basis space (solid lines) from $N_{max} = 4-8$. The most reliable $\hbar\Omega$ value for this extrapolation method is at $\hbar\Omega = 25$ MeV for all states depicted. Experimental (exp.) data are taken from Ref. [13].

resonances. Interestingly, the high-lying $J^\pi = 5^-$ state has a relatively weak $\hbar\Omega$ dependence (compared to states with similar excitation energy); it is also less dependent on N_{max} and may correspond to a narrower resonance.

Note that the conventional wisdom suggests leading configurations for the ground and five lowest-lying levels of ^{14}F (^{14}B) to be formed by the $p_{3/2}$ neutron (proton) and the $s_{1/2}$ or $d_{5/2}$ proton (neutron). Other low-lying states, with the exception of our low-lying 5^- state, involve $p_{1/2}$ and/or $d_{3/2}$ single-particle states.

In Fig. 4 we can also see that the excitation energies obtained with LSO(2) renormalized JISP16 are nearly the same as those obtained with the bare interaction, at least at $N_{max} = 6$. Note that the NCFC results differ significantly from the bare and LSO(2) results, in particular, for the higher excited states with a strong N_{max} dependence; these extrapolated results also tend to have a somewhat weaker dependence on $\hbar\Omega$ than the results in finite basis spaces, and are expected to be more accurate.

Some of the excited states in ^{14}B were observed experimentally. Unfortunately, the spin of most of these states is doubtful or unknown. Overall, the calculated excitation energies appear to be too large compared with the experimental data; in particular, our result for the excited 2^- state, the only excited state with a firm spin assignment, is about 1.5 MeV above the experimental value. However, the spin of the lowest five states agrees with experiment, except for the 2^- and 4^- being interchanged, assuming that the tentative experimental spin assignments are correct. We do not see additional states between 2 and 3 MeV, but this could be related to the fact that all our excitation energies appear to be too large. Also, given the strong dependence on N_{max} of the higher excited states, it is not unlikely that these states will come down further with increasing basis space.

We performed the first theoretical *ab initio* study of the exotic proton-rich nucleus ^{14}F, which has yet to be observed experimentally. Using the NN interaction JISP16, we presented a prediction for the ^{14}F binding energy that is supported by comparing our NCFC results with experimental data for the binding energies of the mirror nucleus ^{14}B and the neighboring nucleus ^{13}O obtained within the same approach in the same basis spaces.

We extended our NCFC extrapolation techniques to evaluate excited states and validated this method by applying it to excited states in ^{6}Li. The spectrum obtained for ^{14}B agrees qualitatively with the limited data, and we made predictions for the spectrum of ^{14}F. More definite information about the excited states in ^{14}B would be helpful. It would also be very interesting to compare our predictions for the ^{14}F binding energy and spectrum with the experimental data that are anticipated soon. Significant differences between our predictions and the experimental results would indicate deficiencies in the NN interaction, JISP16, and/or the role of neglected 3NFs. This would inform future research efforts and, with the inclusion of additional unstable nuclei in the analysis, aid in the eventual determination of the underlying shell structure evolution.

Although NCSM calculations with LSO(2) renormalized interactions generally give reasonable results for the binding energies and spectra in small basis spaces, they do not improve systematically with increasing basis space. In particular, for JISP16 we find that the results for the bare and the LSO(2) renormalized interaction basically coincide for $N_{\max} \geqslant 8$, both for total energies and for excitation energies. It would be worthwhile, although it is a major undertaking, to evaluate the effects of the induced three- and four-body interactions, which should improve the accuracy of the LSO renormalized calculations. Without a thorough study of those effects, however, we prefer the NCFC approach, based on extrapolations of NCSM results with the bare interaction, at least for JISP16.

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