Full Configuration Study of Light No-Core Nuclei with Novel Realistic NN Interaction JISP16

A.M. Shirokov[1,2], J.P. Vary[2], and P. Maris[2]

[1] Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow, 119991 Russia

[2] Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

Abstract. We introduce the no-core full configuration (NCFC) approach and present results for ^{4}He, ^{12}C and ^{14}F with the realistic NN interaction, JISP16. We obtain ground state energies and their uncertainties through exponential extrapolations that we demonstrate are reliable in ^{4}He where fully converged results are obtained. We find ^{12}C is overbound by 1.7 MeV and we predict the yet-to-be-measured binding energy of ^{14}F to be 70.2 ± 3.5 MeV. The extrapolated spectrum of ^{14}F is in reasonable agreement with known features of the ^{14}B spectrum.

1 Introduction and Motivation

The rapid development of *ab-initio* methods for solving finite nuclei has opened the range of nuclear phenomena that can be evaluated to high precision using realistic nucleon-nucleon (NN) and three-nucleon (NNN) interactions, even interactions tied to QCD [1, 2] where renormalization is necessary [3]. Here we present methods for the direct solution of the nuclear many-body problem by diagonalization in a sufficiently large basis space that converged binding energies are accessed — either directly or by simple extrapolation. We do not invoke renormalization. We choose a harmonic oscillator (HO) basis with two basis parameters, the HO energy $\hbar\Omega$ and the many-body basis space cutoff $N_{\max}$, defined below. We assess convergence in this $2D$ parameter space.

Such a direct approach may be referred to as a "No-Core Full Configuration" (NCFC) method. Given the rapid advances in numerical algorithms and computers, as well as the development of realistic non-local NN interactions [4] that facilitate convergence, we are able to achieve converged results, either directly or through extrapolation. That is, we do not need to soften the NN interaction by treating it with an effective interaction formalism. Renormalization formalisms necessarily generate many-body interactions that significantly complicate the theory and are often truncated for that reason. Renormalization without retaining the effective many-body potentials also abandons the variational upper bound characteristic that we prefer to retain. We use a realistic JISP16 NN interaction [4, 5] designed to describe light nuclei without NNN interactions.

We adopt an m-scheme basis approach where the many-body basis states are limited by the imposed symmetries — parity and total angular momentum projection M, as well as by the cutoff in the total oscillator quanta above the minimum for

that nucleus ($N_{\max}$). In natural parity cases, $M = 0$ (or $\frac{1}{2}$) enables the simultaneous calculation of the entire spectrum for that parity and $N_{\max}$. In many light nuclei, we obtain results for the first few increments of $N_{\max}$ and extrapolate calculated observables from a sequence of results obtained with these $N_{\max}$ values.

In our NCFC approach, the input Hamiltonian is independent of $N_{\max}$; the computer requirements for a NCFC calculation are the same as that of the *ab-initio* No Core Shell Model (NCSM) [6] with a 2-body Hamiltonian renormalized to the chosen $N_{\max}$ basis. The NCFC results are obtained by taking the limit of $N_{\max} \to \infty$. Both the NCFC and NCSM approaches guarantee that all observables are obtained free of contamination from spurious center-of-mass (CM) motion effects.

2 Hamiltonian, Basis Selection and Method of Solution

In order to carry out the NCFC calculations, we require a realistic NN interaction that is sufficiently weak at high momentum transfers that we can obtain a reasonable convergence trend. The conventional Lee–Suzuki–Okamoto renormalization procedure of the *ab-initio* NCSM [6] develops effective interactions that provide answers close to experimental observations. However, the convergence trend of the effective interaction sequences with increasing $N_{\max}$ is not uniform and leads to challenges for extrapolation. Therefore, we select the realistic NN interaction, JISP16, that produces spectra and other observables in light nuclei that are in reasonable accord with experiment [4]. We include the Coulomb interaction between the protons.

We cast the many-body problem with the "bare" interaction in the same HO basis and with the same definition of the cutoff as the *ab-initio* NCSM [6]. That is, the many-body finite matrix problem is defined by $N_{\max}$, the maximum number of oscillator quanta shared by all nucleons above the lowest HO configuration for the chosen nucleus. The exact NCFC answer emerges in the limit $N_{\max} \to \infty$. This definition of the cutoff allows us to retain the same treatment of the CM constraint that eliminates spurious CM excitations as in the *ab-initio* NCSM. The Hamiltonian matrix also depends on the HO energy, $\hbar\Omega$.

Our approach satisfies the variational principle and guarantees uniform convergence from above the exact eigenenergy with increasing $N_{\max}$. That is, the results for the energy of lowest state of each spin and parity, at any $N_{\max}$ truncation, are upper bounds on the exact NCFC converged answers and the convergence is monotonic with increasing $N_{\max}$. Our goal is to achieve independence of the two parameters as that is a signal for convergence — the result that would be obtained from solving the same problem in a complete basis.

We employ the code "Many Fermion Dynamics — nuclear" (MFDn) [7] that evaluates the many-body Hamiltonian and obtains the low-lying eigenvalues and eigenvectors using the Lanczos algorithm.

By investigating the calculated binding energies of many light nuclei as a function of the two basis space parameters, we determined that, once we exclude the $N_{\max} = 0$ result, the calculated points represent an exponential convergence pattern. Therefore, we fit an exponential plus constant to each set of results as a function

of $N_{\max}$, excluding $N_{\max} = 0$ at fixed $\hbar\Omega$, using the relation:

$$E_{\mathrm{gs}}(N_{\max}) = a \exp(-cN_{\max}) + E_{\mathrm{gs}}(\infty). \tag{1}$$

3 Extrapolating the Ground State Energy — NCFC Test Cases with ^{4}He

We now investigate the convergence rate for the ground state energy as a function of $N_{\max}$ and $\hbar\Omega$ for ^{4}He where we also achieve nearly exact results by direct diagonalization for comparison. In particular, we present the results and extrapolation analyses for ^{4}He in Figures 1 through 3.

The sequence of curves in Figure 1 for ^{4}He illustrates the trends we encounter in calculations when evaluating the ground state energy with the "bare" JISP16 interaction. Our purpose with ^{4}He is only to illustrate convergence trends. The $N_{\max} = 18$ curve reaches to within 3 keV of the exact answer that agrees with experiment.

Next, we use these ^{4}He results to test our "extrapolation method A" as illustrated in Figure 2. For extrapolation A, we will fit only four calculated points at each value of $\hbar\Omega$. However, in Figure 2 we demonstrate the exponential behavior over the range $N_{\max} = 2{-}16$. Later, we will introduce a variant, "extrapolation method B" in which we use only three successive points for the fit. For extrapolation A, we select the values of $\hbar\Omega$ to include in the analysis by first taking the value at which the minimum (with respect to $\hbar\Omega$) occurs along the highest $N_{\max}$ curve included
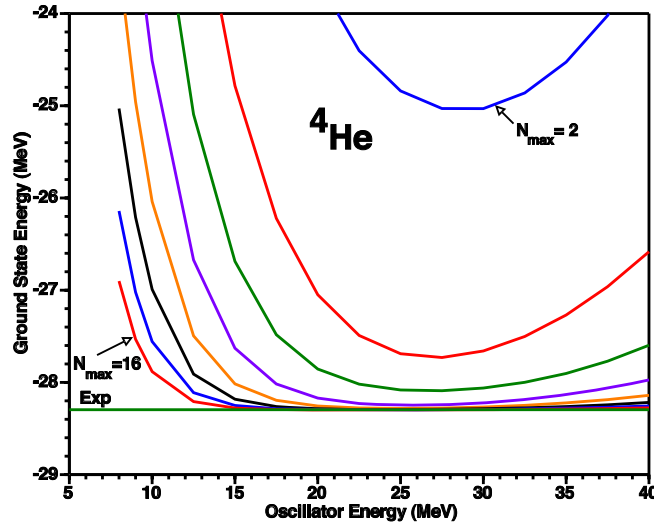

Figure 1. Calculated ground state energy of ^{4}He as function of the oscillator energy, $\hbar\Omega$, for a sequence of $N_{\max}$ values. The curve closest to experiment corresponds to the value $N_{\max} = 16$ and successively higher curves are obtained with $N_{\max}$ decreased by 2 units for each curve.
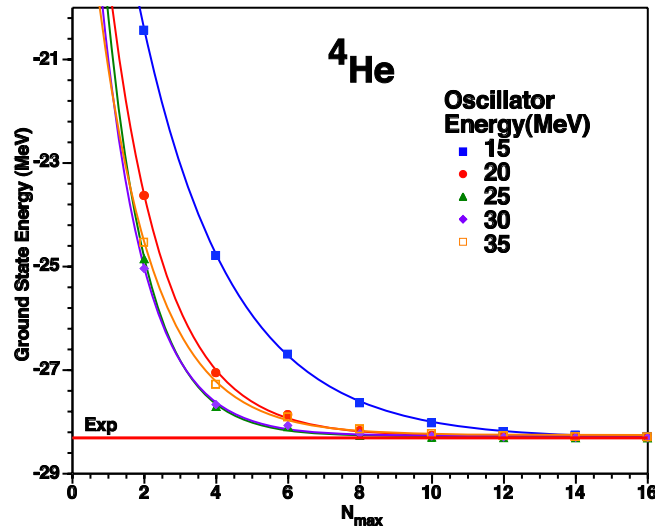
Figure 2. Calculated ground state energy of ^{4}He for $N_{\max} = 2-16$ for JISP16 at selected values of $\hbar\Omega$. Each set of points at fixed $\hbar\Omega$ is fitted by Eq. (1) producing the solid curves. Note the expanded energy scale. Each point is a true upper bound to the exact answer. The asymptotes $E_{\mathrm{gs}}(\infty)$ are the same to within 35 keV of their average value and they span the experimental ground state energy.

in the fit, then taking one $\hbar\Omega$ value lower by 5 MeV and three $\hbar\Omega$ values higher by successive increments of 5 MeV. For heavier systems we take this increment to be 2.5 MeV. Since the minimum occurs along the $N_{\max} = 16$ curve at $\hbar\Omega = 20$ MeV as shown in Figure 1, this produces the 5 curves spanning a range of 20 MeV in $\hbar\Omega$ shown in Figure 2.

We recognize that this window of results in $\hbar\Omega$ values is arbitrary. Our only assurance is that it seems to provide a consistent set of extrapolations in the nuclei examined up to the present time.

For the resulting 5 cases shown in Figure 2, we employ an independent exponential plus constant for each sequence, perform a linear regression for each sequence at fixed $\hbar\Omega$, and observe a small spread in the extrapolants that is indicative of the uncertainty in this method. Note that the results in Figure 2 are obtained with equal weights for each of the points.

For extrapolation A, we will fit sets of 4 successive points due to a desire to minimize the fluctuations due to certain "odd-even" effects. These effects may be interpreted as sensitivity to incrementing the basis space with a single HO state at a time while including two successive basis states affords tradeoffs that yield a better balance in the phasing with the exact solution.

Next, we consider what weight to assign to each calculated point. We argue that, as $N_{\max}$ increases, we are approaching the exact result from above with increasing precision. Hence, the importance of results grows with increasing $N_{\max}$ and this

should be reflected in the weights assigned to the calculated points used in the fitting procedure. With this in mind, we adopt the following strategy: define a chisquare function to be minimized and assign a "sigma" to each calculated result at N_{max} that is based on the change in the calculated energy from the previous N_{max} value. To complete these sigma assignments, the sigma for the first point on the N_{max} curve is assigned a value three times the sigma calculated for the second point on the same fixed-$\hbar\Omega$ trajectory.

As a final element to our extrapolation A strategy, we invoke the minimization principle to argue that all curves of results at fixed $\hbar\Omega$ will approach the same exact answer from above. Thus all curves will have a common asymptote and we use that condition as a constraint on the chisquare minimization.

When we use exponential fits constrained to have a common asymptote and uncertainties based on the local slope, we obtain curves close to those in Figure 2. The differences are difficult to perceive in a graph so we omit presenting a separate figure for them in this case. It is noteworthy that the equal weighting of the linear regression leads to a spread in the extrapolants that is modest.

The sequence of asymptotes for the ^{4}He ground state energy, obtained with extrapolation A, by using successive sets of 4 points in N_{max} and performing our constrained fits to each such set of 4 points, is shown in Figure 3. We employ the independent fits similar to those in Figure 2 to define the uncertainty in our asymptotes. In particular, we define our uncertainty, or estimate of the standard deviation for the constrained asymptote, as one-half the total spread in the asymptotes arising
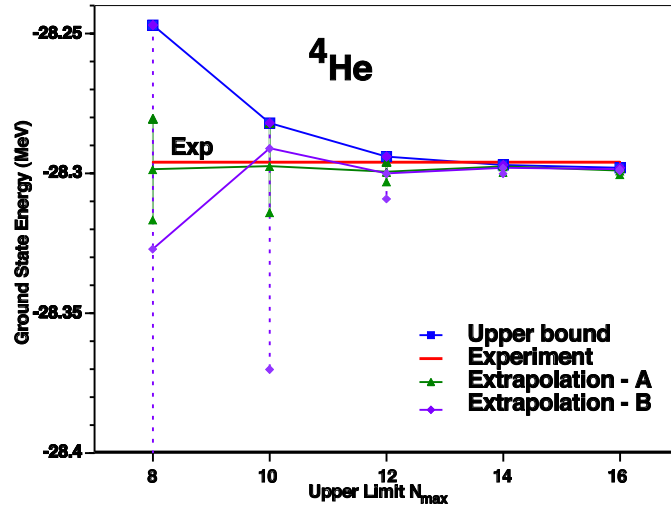

Figure 3. Extracted asymptotes and upper bounds as functions of the largest value of N_{max} in each set of points used in the extrapolation. Four (three) successive points in N_{max} are used for the extrapolation A (B). Uncertainties are determined as described in the text. Note the expanded scale and the consistency of the asymptotes as they fall well within their uncertainty ranges along the path of a converging sequence.

from the independent fits with equal weights for each of the 4 points. In some other nuclei, on rare occasions, we obtain an outlier when the linear regression produces a residual less than 0.999 that we discard from the determination of the total spread. Also, on rare occasions, the calculated upper uncertainty reaches above the calculated upper bound. When this happens, we reduce the upper uncertainty to the upper bound as it is a strict limit.

One may worry that the resulting extrapolation tool contains several arbitrary aspects and we agree with that concern. Our only recourse is to cross-check these choices with solvable NCFC cases as we have done [8]. We seek consistency of the constrained extrapolations as gauged by the uncertainties estimated from the unconstrained extrapolations described above. Indeed, our results such as those shown in Figure 3, demonstrate that consistency. The deviation of any specific constrained extrapolant from the result at the highest upper limit $N_{\max}$ appears well characterized by the assigned uncertainty. We have carried out, and will present elsewhere, a far more extensive set of tests of our extrapolation methods [8].

As we proceed to applications in heavier nuclei, we face the technical limitations of rapidly increasing basis space dimension. In some cases, only three points on the $N_{\max}$ curves may be available so we introduce extrapolation B. Our extrapolation B procedure uses three successive points in $N_{\max}$ to determine the exponential plus constant. We search for the value of $\hbar\Omega$ where the extrapolation is most stable and assign the uncertainty to be the difference in the ground state energy of the highest two points in $N_{\max}$. As expected, since extrapolation B uses less "data" to determine the asymptote, it will have the larger uncertainty. Again, we trim the upper uncertainty, when needed, to conform to the upper bound.

We present the behavior of the asymptotes determined by extrapolations A and B in Figure 3 along with the experimental and upper bound energies. In this case the results are very rapidly convergent at many values of $\hbar\Omega$ producing uncertainties that drop precipitously with increasing $N_{\max}$ as seen in the figure. We note that the uncertainties conservatively represent the spread in the asymptotes since all the extracted asymptotes are consistent with each other within the respective uncertainties. The largest $N_{\max}$ points define the results quoted in Table 1, a ground state overbound by 3 ± 1 keV.

4 Extrapolating the Ground State Energy: NCFC for ^{12}C and ^{14}F

In our investigations of the lightest nuclei [8] we observe a marked correlation between binding energy and convergence rate: the more deeply bound ground states exhibit greater independence of $\hbar\Omega$ at fixed $N_{\max}$. Our physical intuition supports this correlation since we know the asymptotic tails of the bound state wave functions fall more slowly as one approaches a threshold for dissociation. This same intuition tells us to expect Coulomb barriers and angular momenta to play significant roles in this correlation.

We proceed to discuss the ^{12}C results by introducing Figures 4 and 5. The ^{12}C nucleus is the first case for which we have only the extrapolation from the

Table 1. Binding energies of several light nuclei from experiment and theory. The theoretical results are obtained with the JISP16 interaction in NCFC calculations as described in the text. The uncertainties in the rightmost digits of an extrapolation is quoted in parenthesis. We present also variational lower bounds for the binding energies and the uppermost value of $N_{\max}$ used in the quoted extrapolations.

Nucleus/property	Exp	Extrap (A)	Extrap (B)	Lower bound	Max($N_{\max}$)
^{3}H $\|E(\frac{1}{2}^+, \frac{1}{2})\|$ [MeV]	8.482	8.369(1)	8.3695(25)	8.367	18
^{3}He $\|E(\frac{1}{2}^+, \frac{1}{2})\|$ [MeV]	7.718	7.665(1)	7.668(5)	7.663	18
^{4}He $\|E(0^+, 0)\|$ [MeV]	28.296	28.299(1)	28.299(1)	28.298	18
^{6}He $\|E(0^+, 1)\|$ [MeV]	29.269	28.68(12)	28.69(5)	28.473	14
^{6}Li $\|E(1^+, 0)\|$ [MeV]	31.995	31.43(12)	31.45(5)	31.185	14
^{8}He $\|E(0^+, 2)\|$ [MeV]	31.408	29.74(34)	30.05(60)	28.927	12
^{12}C $\|E(0_1^+, 0)\|$ [MeV]	92.162	93.9(1.1)	95.1(2.7)	90.9	8
^{13}O $\|E(\frac{3}{2}^-, \frac{3}{2})\|$ [MeV]	75.556	75.6(2.2)	77.6(2.0)	69.1	8
^{14}B $\|E(2^-, 2)\|$ [MeV]	85.42	83.7(3.1)	85.5(2.0)	76.0	8
^{14}F $\|E(2^-, 2)\|$ [MeV]	?	70.2(3.5)	71.8(2.4)	61.4	8
^{16}O $\|E(0_1^+, 0)\|$ [MeV]	127.619	143.5(1.0)	150 (14)	134.5	8

$N_{\max} = 2-8$ results since the $N_{\max} = 10$ basis space, with a dimension of 7,830,355,795, is beyond our present capabilities. Thus, in order to illustrate the details of our uncertainties, we depict in Figure 5 the linear regression analyses of
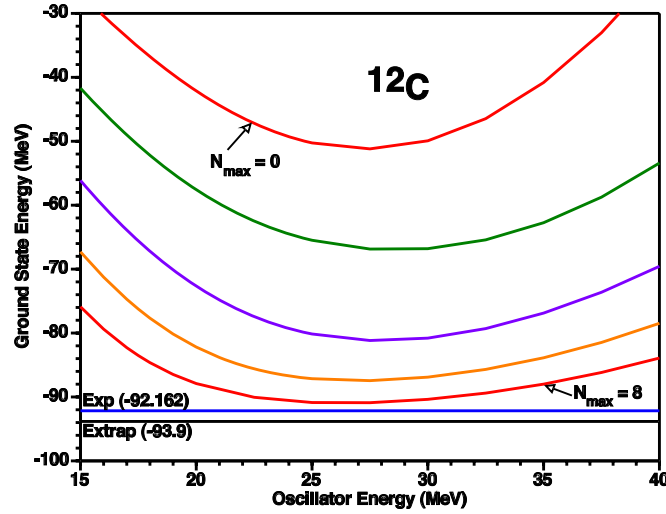

Figure 4. Calculated ground state energy of ^{12}C as function of the oscillator energy, $\hbar\Omega$, for selected values of $N_{\max}$. The curve closest to experiment corresponds to the value $N_{\max} = 8$ and successively higher curves are obtained with $N_{\max}$ decreased by 2 units for each curve.
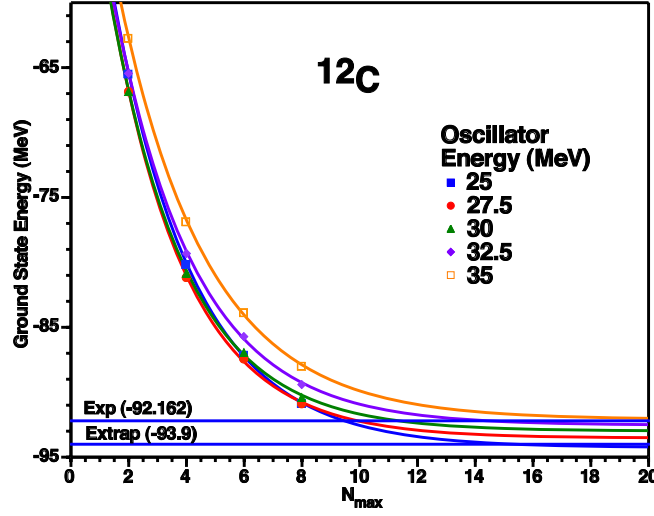
Figure 5. Calculated ground state energy of ^{12}C for $N_{max} = 2-8$ at selected values of $\hbar\Omega$ as described in the text. For each $\hbar\Omega$ the data are fit to an exponential plus a constant, the asymptote. The figure displays the experimental ground state energy and the common asymptote obtained in extrapolation A.

our results spanning the minimum in $\hbar\Omega$ obtained at $N_{max} = 8$. Extrapolation A produces overbinding by about 1.7 MeV.

Our next example is ^{14}F, an exotic neutron-deficient nucleus, the first observation of which is expected in an experiment planned in the Cyclotron Institute at Texas A&M University. In this case, we also attain the results up through $N_{max} = 8$ presented in Figure 6. The $N_{max} = 8$ basis includes 1,990,061,078 states. The results of extrapolation B are shown in the figure by crosses for different $\hbar\Omega$ values. In the case of extrapolation A, we obtain the binding energy prediction of 70.2 ± 3.5 MeV (shaded area in Figure 6) which is seen to be in a good correspondence with extrapolation B that provides the binding energy of 71.8 ± 2.4 MeV with a smaller value of estimated uncertainty. It is interesting that, contrary to our NCFC approach, the trend of the conventional effective interaction calculations of the binding energy is misleading in this case: the minimum of the respective $\hbar\Omega$ dependence is seen from Figure 6 to shift up with increasing N_{max} indicating the development of a shallow minimum at $N_{max} = 6$ around $\hbar\Omega = 12.5$ MeV; the ground state energy at this minimum is above the upper bound resulting from the variational principle and calculations with the "bare" JISP16 interaction. The reliability of the ^{14}F results is supported by calculations of the binding energy of the mirror nucleus ^{14}B (see Table 1).

We performed also calculations of the excited states in ^{14}F. The results obtained with $\hbar\Omega = 25$ MeV in the range of N_{max} values of 0–8, are presented in Figure 7. We performed the extrapolation B for the energies of these states. The respective excitation energies, i.e. the differences between the extrapolated energies and the
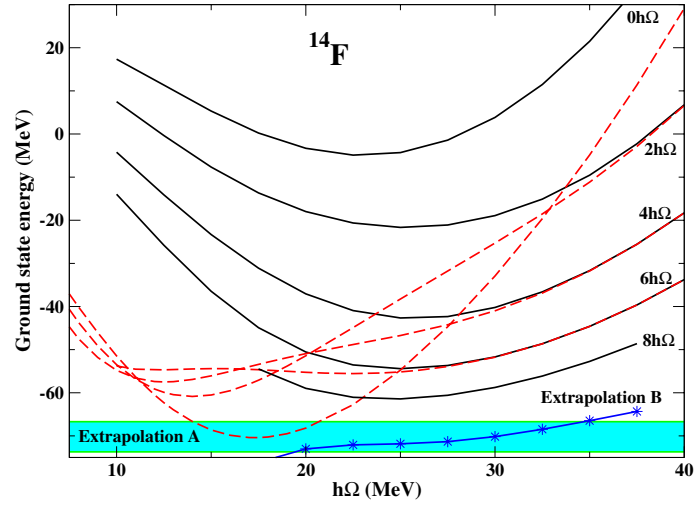
Figure 6. Calculated ground state energy of ^{14}F for $N_{\mathrm{max}} = 0-8$ with "bare" (solid lines) and effective (dashed lines) JISP16 interaction as function of the oscillator energy $\hbar\Omega$. Shaded area shows a confidence region of extrapolation A predictions, stars depict predictions by extrapolation B for individual $\hbar\Omega$ values.
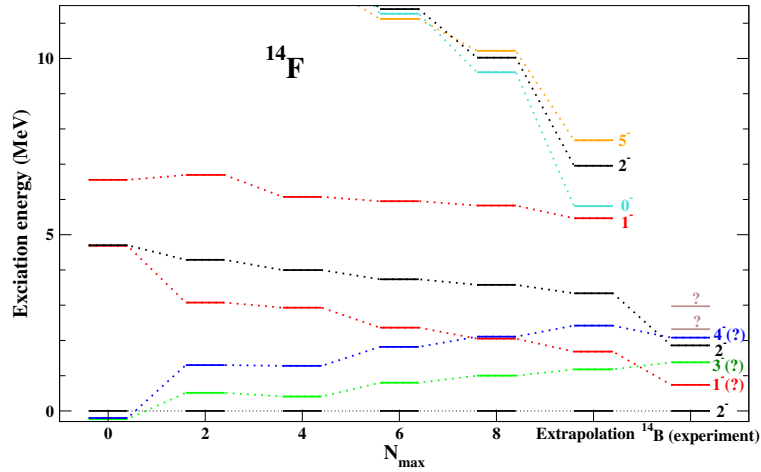

Figure 7. The ^{14}F spectrum obtained with $N_{\mathrm{max}} = 0-8$ and $\hbar\Omega = 25$ MeV and by the extrapolation of the excited states in comparison with the spectrum of the mirror nucleus ^{14}B.

extrapolated ground state energy, are also shown in the figure. The ^{14}F spectrum is seen to be in a reasonable agreement with the spectrum of the mirror nucleus ^{14}B. However we should note here that the spin assignments of nearly all states in the ^{14}B spectrum are doubtful.

5 Conclusions and Outlook

We present in Table 1 a summary of the extrapolations performed with methods introduced here and compare them with the experimental results. In all cases, we used the calculated results to the maximum $N_{\max}$ available with the bare JISP16 interaction. Our overall conclusion is that these NCFC results demonstrate sufficient convergence achieved for ground state energies of light nuclei allowing extrapolations to the infinite basis limit and estimations of their uncertainties. These convergence properties are provided by the unique features of the JISP16 NN interaction. The convergence rate reflects the short range properties of the nuclear Hamiltonian. Fortunately, new renormalization schemes have been developed and applied that show promise for providing suitable nuclear Hamiltonians based on other interactions with good convergence properties within the NCFC method [9]. Additional work is needed to develop the corresponding NNN interactions. Also, further work is in progress to extrapolate the RMS radii.

References

1. C. Ordonez, L. Ray, and U. van Kolck, Phys. Rev. Lett. **72**, 1982 (1994); Phys. Rev. C **53**, 2086 (1996).
2. D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001(R) (2003).
3. P. Navrátil, V. G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, Phys. Rev. Lett. **99**, 014315 (2007).
4. A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, Phys. Lett. B **644**, 33 (2007); A. M. Shirokov, J. P. Vary, A. I. Mazur, S. A. Zaytsev and T. A. Weber, Phys. Lett. B **621**, 96 (2005).
5. Software providing the matrix elements of the JISP16 NN interaction may be downloaded from `http://nuclear.physics.iastate.edu`.
6. P. Navrátil, J. P. Vary and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000); Phys. Rev. C **62**, 054311 (2000).
7. J. P. Vary, "The Many Fermion Dynamics Shell Model Code," Iowa State University, 1992 (unpublished); J. P. Vary and D. C. Zheng, *ibid* 1994 (unpublished); sample runs of the code may be performed by accessing `http://nuclear.physics.iastate.edu`.
8. P. Maris, J. P. Vary, and A. M. Shirokov, arXiv: 0808.3420 (2008).
9. S. K. Bogner, R. J. Furnstahl, P. Maris, R. J. Perry, A. Schwenk, and J. P. Vary, Nucl. Phys. A **801**, 21 (2008).