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NN Interaction JISP16: Current Status and Prospect

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Abstract. We discuss realistic nonlocal *NN* interactions of a new type — *J*-matrix Inverse Scattering Potential (JISP). In an *ab exitu* approach, these interactions are fitted to not only two-nucleon data (*NN* scattering data and deuteron properties) but also to the properties of light nuclei without referring to three-nucleon forces. We discuss recent progress with the *ab initio* No-core Shell Model (NCSM) approach and respective progress in developing *ab exitu* JISP-type *NN*-interactions together with plans of their forthcoming improvements.

Significant progress was achieved within the last decade in *ab initio* studies of light nuclei. Nowadays, due to increased computing power and novel techniques, *ab initio* approaches like the No-core Shell Model (NCSM) [1], the Green's function Monte Carlo [2] and the coupled-cluster theory [3] are able to reproduce properties of a large number of atomic nuclei with mass up to $A = 16$ and can be extended for heavier nuclei.

The *ab initio* methods require a reliable realistic strong interaction providing an accurate description of *NN* scattering data and high-quality predictions for binding energies, spectra and other observables in light nuclei. A number of meson-exchange potentials sometimes supplemented with phenomenological terms to achieve high accuracy in fitting *NN* data (CD-Bonn [4], Nijmegen [5], Argonne [6]) have been developed that should be used together with modern *NNN* forces (Urbana [7,8], Illinois [9], Tucson–Melbourne [10,11]) to reproduce properties of many-body nuclear systems. On the other hand, one sees the emergence of *NN* and *NNN* interactions with ties to QCD [12–15].

Three-nucleon forces require a significant increase of computational resources needed to diagonalize a many-body Hamiltonian matrix since the *NNN* interaction increases the number of non-zero matrix elements approximately by a factor of 30 in the case of *p*-shell nuclei. As a result, one needs to restrict the basis space in many-body calculations when *NNN* forces are involved that makes the predictions less reliable. *Ab initio* many-body studies benefit from the use of recently developed purely two-nucleon interactions of INOY (Inside Nonlocal Outside Yukawa) [16,17] and JISP (*J*-matrix Inverse Scattering Potential) [18–21] types fitted not only to the *NN* data but also to binding energies of $A = 3$ and heavier nuclei. At the fundamental level, these *NN* interactions are supported by the work of Polyzou and Glöckle who demonstrated [22] that a realistic *NN* interaction is equivalent at the $A = 3$ level to some $NN + NNN$ interaction where the new *NN* force is related to the initial one through a phase-equivalent transformation (PET). It seems reasonable then to exploit this freedom and work to minimize the need for the explicit introduction of three and higher body forces. Endeavors along these lines have resulted in the design of INOY and JISP strong interaction models.

We discuss here the progress in development of the JISP *NN* interactions and related progress in NCSM studies of light nuclei.

1 The original JISP16

The *J*-matrix inverse scattering approach was suggested in Ref. [23]. It was further developed and used to design a high-quality JISP *NN* interaction in Ref. [18]. A nonlocal interaction obtained in this approach is in the form of a matrix in the oscillator basis in each of the *NN* partial waves. To reproduce scattering data in a wider energy range, one needs to increase the size of the potential matrix and/or the $\hbar\Omega$ parameter of oscillator basis. From the point of view of shell model applications, it is desirable however to reduce the size of potential matrices and to use $\hbar\Omega$ values in the range of few tens of MeV. A compromise solution is to use $\hbar\Omega = 40$ MeV with $N_{\max} = 9$ truncation of potential matrices [18], i.e., we use potential matrices of the rank $r = 5$ in *s* and *p* *NN* partial waves, $r = 4$ matrices in *d* and *f* partial waves, etc.; in the case of coupled waves, the rank of the potential matrix is a sum of of the respective ranks, e.g., the rank of the coupled *sd* wave matrix is $r = 5 + 4 = 9$. The $N_{\max} = 9$ truncated JISP interaction with $\hbar\Omega = 40$ MeV provides an excellent description of *NN* scattering data with χ^2/datum = 1.03 for the 1992 *np* data base (2514 data), and 1.05 for the 1999 *np* data base (3058 data) [24].

PETs originating from unitary transformations of the oscillator basis proposed in [25,26], give rise to ambigui-

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Table 1. JISP6 and JISP16 deuteron property predictions in comparison with the ones obtained with various realistic potentials.

Potential	E_d, MeV	d state probability, %	rms radius, fm	Q, fm^2	As. norm. const. $\mathscr{A}_s$, fm$^{-1/2}$	$\eta = \frac{\mathscr{A}_d}{\mathscr{A}_s}$
JISP6, JISP16	−2.224575	4.1360	1.9647	0.2915	0.8629	0.0252
Nijmegen-II	−2.224575	5.635	1.968	0.2707	0.8845	0.0252
AV18	−2.224575	5.76	1.967	0.270	0.8850	0.0250
CD–Bonn	−2.224575	4.85	1.966	0.270	0.8846	0.0256
Nature	−2.224575(9)	—	1.971(6)	0.2859(3)	0.8846(9)	0.0256(4)

ties of interaction obtained in the J-matrix inverse scattering approach. These ambiguities are eliminated at the first stage by postulating the simplest tridiagonal form of the NN interaction in uncoupled and quasi-tridiagonal form in coupled NN partial waves [18]. At the next stage, PETs are used to fit the JISP interaction to various nuclear properties. First of all, the *sd* component of the NN interaction is modified with the help of PETs to reproduce the deuteron quadrupole moment Q and rms radius without violating the excellent description of scattering data. The deuteron property predictions obtained with JISP and other interaction models are listed in Table 1. It is worth noting here that the deuteron binding energy E_d and asymptotic normalization constants $\mathscr{A}_s$ and $\mathscr{A}_d$ are used as an input in the inverse scattering approach and are not affected by PETs.

After that we employ PETs in other NN partial waves attempting to improve the description of binding energies and spectra of light nuclei in NCSM calculations. Following this *ab exitu* route, the JISP6 NN interaction fitted to properties of nuclei with masses $A \leq 6$, was proposed [19]. It was found out later that JISP6 strongly overbinds nuclei with $A \geq 10$. Therefore a new fit of PET parameters was performed that resulted in the JISP16 interaction [20] fitted to nuclei with masses up through $A = 16$. After discussing methods used in the fit of the JISP16 interaction and results obtained with it, we shall concentrate on some drawbacks of this interaction revealed due to the recent progress in the NCSM approach [27] and attainment of larger basis spaces in calculations, and propose its new refined version JISP16$_{2010}$.

Our fitting procedure was one of 'trial-and-error' where we worked with only a few partial waves that we thought might be important for light nuclei. We fitted only the excitation energies of the lowest ^{6}Li levels and the ^{6}Li and ^{16}O binding energies. To save time, we performed the NCSM calculations in small enough $N_{\max}\hbar\Omega$ basis spaces (up to $N_{\max} = 10$ for ^{6}Li and up to $N_{\max} = 4$ for ^{16}O) using the effective interaction obtained from the original 'bare' inverse scattering potential by means of the Lee–Suzuki–Okamoto (LSO) renormalization procedure [28]. The renormalization procedure was truncated at the two-body cluster level — i. e. induced three-body, four-body, etc., contributions are neglected; hence we refer to these calculations as LSO(2) renormalized. The variational principle holds for the bare interaction results, but not for results obtained with the LSO(2) renormalized interaction. Conventional wisdom suggests that the minimum with respect to $\hbar\Omega$ of the ground state energies obtained with the LSO(2) renormalized interaction provides the best estimate of the actual ground state energy; furthermore, this minimum increases with increasing $N_{\max}$ in a number of nuclei, at least for relatively small basis spaces. It was therefore believed that this minimum provides a reasonable lower bound for the actual ground state energy. On the other hand the minimum obtained with the bare interaction provides us with a strict upper bound, because of the variational principle. After obtaining a reasonable description of the lowest ^{6}Li levels and the ^{6}Li and ^{16}O binding energies, we checked that the binding energies and spectra of all the remaining s and p shell nuclei are well-described in similarly small model spaces.

Table 2. Binding energies (in MeV) of nuclei obtained with LSO(2) renormalized JISP16 ("effective interaction", from Ref. [20]), and variational lowerbounds from more recent calculations, generally obtained in larger model spaces than was feasible in 2006, when JISP16 was developed.

Nucleus	Nature	LSO renormalized from Ref. [20]	$N_{\max}$	Variational lowerbound	$N_{\max}$
^{3}H	8.482	8.496	14	8.367	20
^{3}He	7.718	7.797	14	7.663	20
^{4}He	28.296	28.374	14	28.299	18
^{6}He	29.269	28.32	12	28.616	16
^{6}Li	31.995	31.00	12	31.340	16
^{7}Li	39.245	37.59	10	37.954	12
^{7}Be	37.600	35.91	10	36.273	12
^{8}Be	56.500	53.40	8	53.731	10
^{9}Be	58.165	54.63	8	53.577	8
^{9}B	56.314	52.53	8	51.308	8
^{10}Be	64.977	61.39	8	60.596	8
^{10}B	64.751	60.95	8	60.455	8
^{10}C	60.321	56.36	8	55.264	8
^{11}B	76.205	73.0	6	69.182	6
^{11}C	73.440	70.1	6	66.060	6
^{12}B	79.575	75.9	6	71.190	6
^{12}C	92.162	91.0	6	92.814	10
^{12}N	74.041	70.2	6	64.539	6
^{13}B	84.453	82.1	6	73.527	6
^{13}C	97.108	96.4	6	93.208	6
^{13}N	94.105	93.1	6	89.690	6
^{13}O	75.558	72.9	6	69.066	8
^{14}C	105.285	106.0	6	106.853	8
^{14}N	104.659	106.8	6	109.136	8
^{14}O	98.733	99.1	6	99.337	8
^{15}N	115.492	119.5	6	114.409	6
^{15}O	111.956	115.8	6	110.139	6
^{16}O	127.619	133.8	6	134.494	8

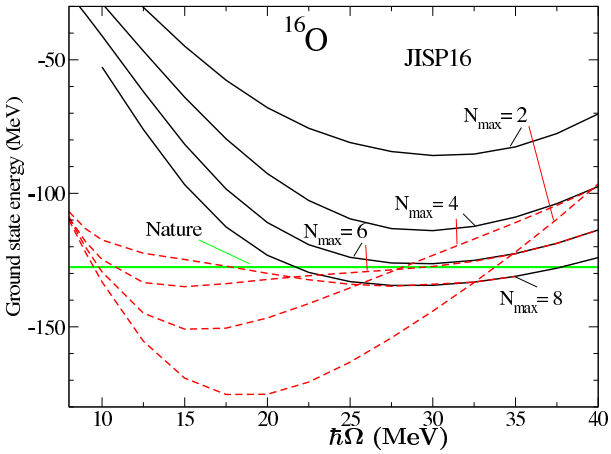

Fig. 1. Results for the ground state energy of ^{16}O with bare (solid) and LSO(2) renormalized (dashed) JISP16 interaction as a function of the oscillator parameter $\hbar\Omega$. When JISP16 was developed [20], the largest model space calculations where $N_{\max} = 6$.

The results presented in Table 2 are obtained in the *ab initio* NCSM calculations with the obtained *NN* interaction, the *ab exitu* JISP16, in larger model spaces. This description of the binding energies is somewhat worse than the one obtained during the fit in smaller model spaces, but is still very reasonable. However, moving to larger model spaces revealed that the convergence of the LSO(2) renormalized JISP16 interaction is not as uniform as suggested by conventional wisdom. In particular for a number of heavier nuclei with $A \geq 12$, the current variational upper bound tends to be lower than our best estimates 3 years ago.

We illustrate this issue by the ^{16}O ground state energy calculations in Fig. 1. The solid curves are our NCSM results with the bare interaction JISP16. The variational principle holds for the bare interaction results; hence these curves form a strict upper bound for the ground state energy. The dashed curves in Fig. 1 were obtained in the more conventional NCSM calculations with the LSO(2) renormalized interaction derived from the initial bare interaction JISP16. For the series of calculations with $N_{\max} = 0$ (not shown), 2, 4, and 6, the minimum of these dashed curves increases with model spaces, and at $N_{\max} = 6$ this minimum is only slightly below the corresponding minimum obtained with the bare interaction (-133.8 MeV and -126.2 MeV respectively). However, the $N_{\max} = 8$ curves for the LSO(2) and bare interaction (dashed and solid curves) clearly demonstrate that with the LSO(2) renormalized interaction does not converge uniformly to the infinite basis space results, nor does it necessarily produce a lower bound.

Similar trends were found for most of the *p* shell nuclei: the LSO(2) renormalized (or effective) interactions produce results which are neither an upper bound nor a lower bound, and the approach to the infinite basis space is non-monotonic. Hence the convergence pattern of the effective interaction results is difficult to assess. Nevertheless, in small model spaces they do give a reasonable estimate of the actual binding energies. As such, the LSO procedure is very useful, in particular for interactions that converge only at very large model spaces, such as N3LO, CD-Bonn, or Argonne. However, JISP16 is a very soft interaction, and the results with the bare interaction converge rapidly, making it unnecessary to use the LSO renormalization techniques for nuclei up to $A \sim 16$. Indeed, this is confirmed by the fact that for large values of $\hbar\Omega$, the bare and LSO(2) renormalized interaction lead to identical results, and that the $\hbar\Omega$ range over which the results from the bare and LSO(2) renormalized interactions coincide increases with the basis space.

The nuclear Hamiltonian based on the realistic nonlocal *NN* interaction JISP16, seems from Table 2 to reproduce well the binding energies of nuclei with $A \leq 16$. The lowest state of natural parity has the correct total angular momentum in each nucleus studied. Furthermore, it reproduces the spectra of ^{6}Li and ^{10}B [20], which are known to be sensitive to an explicit *NNN* interaction. This feature of incorporating by a purely two-body interaction of what is conventionally believed to be a 3-body force effect, is attributed to the fact that JISP16 is a nonlocal interaction. We also note here that JISP16 provides a good description of the ^{6}Li quadrupole moment Q [20] (see also Table 8 below) that is a recognized challenge due to a delicate cancellation between deuteron quadrupole moment and the *d* wave component of the α–*d* relative wave function.

2 Extrapolation to infinite model space: ^{14}F ground state

Recently we introduced an *ab initio* No-Core Full Configuration (NCFC) approach [27,29], 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 predictions for binding energies and to evaluate their numerical uncertainties. We use two extrapolation methods: a global extrapolation based on the results obtained in four successive basis spaces with five $\hbar\Omega$ values from a 10 MeV interval (extrapolation A); and extrapolation B based on the results obtained at various fixed $\hbar\Omega$ values in three successive basis spaces and defining the most reliable $\hbar\Omega$ value for the extrapolation. These extrapolations provide consistent results and were carefully tested in a number of light nuclei where a complete convergence can be achieved [27].

The NCFC approach was used recently [30] for the first *ab initio* study of the exotic proton-excess nucleus ^{14}F. The first experimental results regarding this four proton excess isotope will be available soon from Cyclotron Institute at Texas A&M University [31]. The largest calculations were performed in the $N_{\max}\hbar\Omega$ basis space with $N_{\max} = 8$, which for this nucleus contains 1,990,061,078 basis states with total magnetic projection $M = 0$ and natural parity (negative). The determination of the lowest ten to fifteen eigenstates of the sparse Hamiltonian matrix, for each oscillator parameter $\hbar\Omega$, requires 2 to 3 hours on 7,626 quad-core compute nodes at the Jaguar supercomputer at ORNL.

We show our complete results for the ^{14}F ground state energy in Fig. 2. The solid curves are our NCSM results

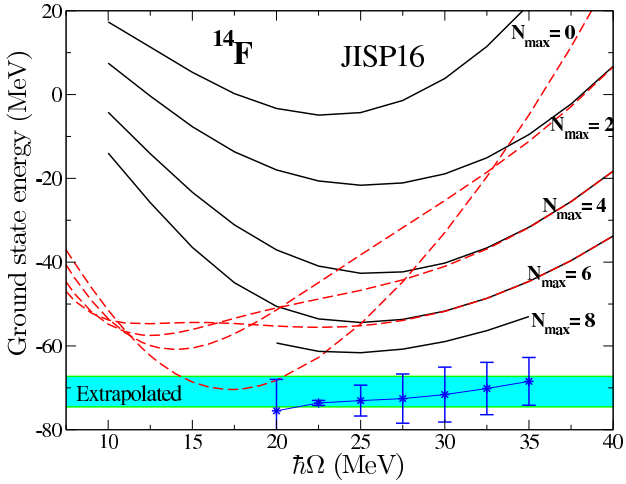

Fig. 2. Results for the ground state energy of ^{14}F with bare (solid) and effective (dashed) JISP16 interaction as a function of the oscillator parameter $\hbar\Omega$. The shaded area demonstrates the global extrapolation A for the binding energy and its uncertainty; the extrapolation B at fixed $\hbar\Omega$ is given by stars with its uncertainties indicated by the error bars. The most reliable $\hbar\Omega$ value for this extrapolation method is at $\hbar\Omega$ = 25 MeV for ^{14}F.

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. 2 are obtained in NCSM calculations with effective *NN* interactions. Again, these results obtained in extremely large NCSM basis spaces and verified by the new basis-space independent *ab initio* NCFC method, reveal some drawbacks of the effective interaction approach that was used in the JISP16 fit to binding energies of light nuclei.

By comparing the bare and effective interaction results in Fig. 2, we observe that the tendency of the LSO(2) 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 effective interaction 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 $N_{\max}$. We see the same convergence pattern in ^{16}O (see Fig. 1) and other *p* shell nuclei. For these reasons, we did not perform expensive $N_{\max}$ = 8 effective interaction calculations for ^{14}F.

We present in Fig. 2 and in Table 3 the results of NCFC extrapolations A and B. Combining both extrapolation methods suggests a binding energy of 72 ± 4 MeV for ^{14}F. Ironically, the minimum of the effective interaction calculations in the smallest $N_{\max}$ = 0 basis space 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 [32]. This value agrees with our prediction of 86 ± 4 MeV. We also performed NCFC calculations of the neighboring nucleus ^{13}O using basis

Table 3. NCFC predictions for the ground state energies (in MeV) of ^{13}O, ^{14}B and ^{14}F based on NCSM calculations with JISP16 in up to $N_{\max}$ = 8 basis spaces. We include in parentheses an estimate of the accuracy of the extrapolations A and B. Experimental data are taken from Ref. [32].

Nucleus	Extrap. A	Extrap. B	Experiment
^{13}O	−75.7(2.2)	−77.6(3.0)	−75.556
^{14}B	−84.4(3.2)	−86.6(3.8)	−85.423
^{14}F	−70.9(3.6)	−73.1(3.7)	—

spaces up to $N_{\max}$ = 8. The calculated binding energy of 77 ± 3 MeV also agrees with the experimental value of 75.556 MeV [32].

We note that a good description of both ^{14}F and ^{13}O in the same approach is important in order to have a description of ^{14}F consistent with the experiment in which ^{14}F will be produced in the ^{13}O + *p* reaction. In this way, any experimentally observed resonances can be directly compared with the difference of our predictions for the ^{14}F and ^{13}O energies. In this respect it is interesting to note that although the total energies of the extrapolations A and B differ by about 2 MeV, the differences between 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.)

3 Extrapolation to infinite model space: Excitation spectra

It is also very interesting to calculate 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 above 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.

To verify this approach to calculate the NCFC excitation energies, we apply it to the spectrum of ^{6}Li nucleus, see Table 4. 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 4 with the extrapolations based on calculations in basis spaces up to $N_{\max}$ = 8, i. e. 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

Table 4. Predictions for the ^{6}Li ground state E_{gs} and excitation energies E_x (in MeV) obtained in different basis spaces with JISP16. For extrapolations A and B we include in parentheses an estimate of the accuracy of the total energies; for the effective interaction ($V_{\rm eff}$), we present the spread in excitation energy for $\hbar\Omega$ variations from 12.5 to 22.5 MeV. Experimental data (in MeV) are taken from Ref. [33].

	Extrap. A	Extrap. B	$V_{\rm eff}$	Extrap. A	Extrap. B	$V_{\rm eff}$	Experiment	
$E(J^\pi,T)$	$N_{\rm max}=2-8$	$N_{\rm max}=4-8$	$N_{\rm max}=6$	$N_{\rm max}=10-16$	$N_{\rm max}=12-16$	$N_{\rm max}=14$	Energy	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	$24\cdot10^{-3}$
$E_x(0^+,1)$	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	$8.2\cdot10^{-6}$
$E_x(2^+,0)$	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

Table 5. Predictions for the ^{14}F and ^{14}B excitation energies E_x (in MeV) based on NCSM calculations with JISP16 in up to $N_{\rm max}=8$ basis spaces. See Table 4 for details. Experimental data (in MeV) are taken from Ref. [32].

	Ab initio NCFC and effective interaction NCSM calculations with JISP16						Experiment	
	^{14}F			^{14}B			^{14}B	
$E(J^\pi,T)$	Extrap. A	Extrap. B	$V_{\rm eff}$, , $N_{\rm max}=6$	Extrap. A	Extrap. B	$V_{\rm eff}$, $N_{\rm max}=6$	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^-)	0.74(4)
$E_x(3^-,2)_1$	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(3)
$E_x(2^-,2)_2$	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(7)
$E_x(4^-,2)_1$	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(5)
							?	2.32(4)
							?	2.97(4)
$E_x(1^-,2)_2$	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		

$N_{\rm max}=16$ results is generally much smaller than the estimated uncertainties in the total energies of the $N_{\rm max}=8$ 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.

The two lowest excited states in ^{6}Li are narrow resonances. Our predictions for these states obtained by extrapolations A and B and with effective interaction, agree very well with experiment. The bare and effective interaction excitation energies of these states show very little dependence on $\hbar\Omega$.

On the other hand, the three higher excited states have a much larger width, see Table 4. Our calculations for these broad resonances show a significant dependence on both $\hbar\Omega$ and $N_{\rm max}$, in particular for the excited $(1^+,0)_2$ state which has the largest width. The extrapolation B to infinite model space reduces but does not eliminate completely 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 [34], and that the slope of the $\hbar\Omega$ dependence increases with the width of the resonance. 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 effective 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 effective interaction are often quite stable with $N_{\rm max}$. However, it is important to realize that this does not necessarily mean that these excitation energies are numerically converged: they can be $\hbar\Omega$-dependent. The dependence of the excitation energies on $\hbar\Omega$ decreases slowly with increasing $N_{\rm max}$, as seen in Table 4. In fact, the excitation energies obtained with effective interaction based on JISP16 are nearly the same as those obtained with the bare JISP16 interaction. For most states, the NCFC provides better results for the excitation energies, with less basis space dependence than the effective interaction NCSM calculations in finite basis spaces. Nevertheless, we can employ the effective interaction to obtain estimates of the binding and excitation energies when only small basis spaces are attainable and the NCFC extrapolations are impossible.

We summarize our results for the spectra of ^{14}F and ^{14}B in Table 5. The excitation energies are obtained as a difference between the extrapolated total energies of the excited

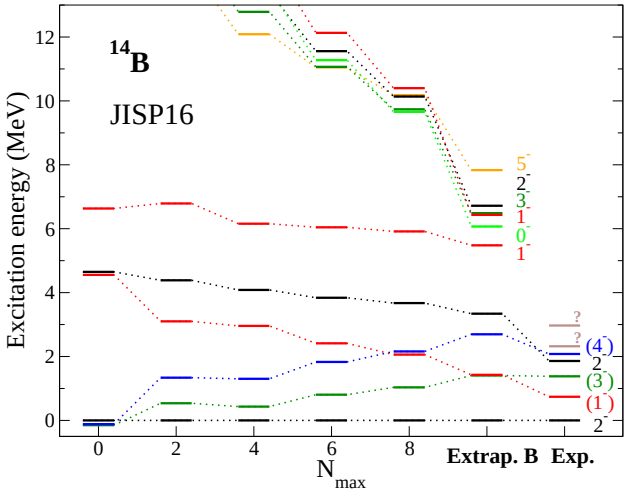

Fig. 3. Negative parity ^{14}B spectrum obtained with bare JISP16 interaction at fixed $\hbar\Omega = 25$ MeV in successive basis spaces, and extrapolated to infinite basis space using Extrapolation B. Experimental data are taken from Ref. [32].

state and that of the ground state (see Table 3). 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. We present in Fig. 3 the ^{14}B results and we note that the behavior of the ^{14}F states is similar. There are five low-lying excited states with excitation energies showing a weak dependence, within about a 1.5 MeV range, on the basis space as $N_{\max}$ increases from 2 to 8. Then there are numerous higher excited states which 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 appear at excitation energies comparable to the other low-lying excited states. The lowest five excited states have a weak dependence on $\hbar\Omega$, whereas the higher excited states depend strongly on it and this strong $\hbar\Omega$ dependence is manifested in larger global extrapolation A uncertainties obtained as a spread of extrapolated results at different $\hbar\Omega$ values. 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 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.

The excitation energies of the lowest five and the high-lying $J^\pi = 5^-$ state obtained with effective interaction are less $\hbar\Omega$-dependent than the other states shown and are consistent with the NCFC extrapolations. For the higher excited states, the NCFC results differ significantly from the effective interaction predictions; 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, our predicted excitation energies appear to be too large when compared with the experimental data; in particular our prediction 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. 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.

4 Towards a renewed JISP16

As we have seen above, the effective interaction approach used in the fitting of the JISP16 interaction, can be misleading in evaluating binding energies of nuclei. The new *ab initio* NCFC aproach provides much more reliable predictions for bindings. Therefore the results presented in Table 2 should be reevaluated using extrapolations A and B. The NCFC binding energies of some nuclei obtained with JISP16 are presented in Table 6. The NCFC approach clearly reveals a deficiency of the JISP16 interaction: it overbinds essentially nuclei with mass $A \geq 14$ and $N \sim Z$.

These deficiencies of the NN interaction can be addressed by a new fit of the PET parameters defining JISP interaction based on the NCFC calculations. Such a fit is much more complicated since it requires calculations in a number of successive basis spaces for each nucleus and each set of parameters. The renewed NN interaction obtained in this fit which we refer to as JISP16$_{2010}$, is fixed by the set of PET rotation parameters listed in Table 7 (the definition of PET rotation parameters ϑ can be found in Refs. [18, 19]). The JISP16 and JISP16$_{2010}$ interactions are characterized by the same ϑ value in coupled sd partial waves; hence both interactions predict the same deuteron properties (see Table 1). All the remaining ϑ values listed in Table 7 differ between JISP16$_{2010}$ and JISP16. We note also that the JISP16 interaction was defined only in the NN partial waves with total momenta $J \leq 4$ while the JISP16$_{2010}$ interaction is extended to all partial waves with $J \leq 8$. The description of NN scattering data by JISP16$_{2010}$ and JISP16 interactions is the same since they are related by phase-equivalent transformations.

We compare binding energies obtained with JISP16 and JISP16$_{2010}$ interactions in Table 6. It is seen that the new interaction essentially improves the description of the p shell nuclei. In particular, JISP16$_{2010}$ provides nearly ex-

Table 6. Binding energies (in MeV) of some nuclei obtained with JISP16 and JISP16$_{2010}$ *NN* interactions by extrapolations A and B; the $N_{\max}$ columns show the largest model space used for the extrapolations.

		JISP16			JISP16$_{2010}$		
Nucleus	Experim.	Extrap. A	Extrap. B	$N_{\max}$	Extrap. A	Extrap. B	$N_{\max}$
^{3}H	8.482	8.369 ± 0.001	8.3695 ± 0.0025	18	8.369 ± 0.010	$8.367^{+0.012}_{-0.007}$	14
^{3}He	7.718	7.665 ± 0.001	7.668 ± 0.005	18	7.664 ± 0.011	7.663 ± 0.008	14
^{4}He	28.296	28.299 ± 0.001	28.299 ± 0.001	18	28.294 ± 0.002	$28.294^{+0.002}_{-0.001}$	14
^{8}He	31.408	29.69 ± 0.69	29.29 ± 0.96	10	30.30 ± 0.46	$29.99^{+1.31}_{-1.06}$	10
^{6}Li	31.995	31.47 ± 0.09	31.48 ± 0.03	16	31.33 ± 0.16	31.34 ± 0.07	14
^{10}B	64.751	63.1 ± 1.2	63.7 ± 1.1	8	62.6 ± 1.4	63.4 ± 1.5	8
^{12}C	92.162	93.9 ± 1.1	95.1 ± 2.7	8	91.1 ± 1.3	92.3 ± 2.9	8
^{14}C	105.284	112.1 ± 2.1	114.3 ± 6.0	8	102.5 ± 1.6	104.8 ± 3.6	8
^{14}N	104.659	114.2 ± 1.9	115.8 ± 5.5	8	102.7 ± 1.5	104.7 ± 3.1	8
^{16}O	127.619	143.5 ± 1.0	150 ± 14	8	126.7 ± 3.1	129.6 ± 6.1	8

Table 7. PET rotation parameters ϑ in various *NN* partial waves defining the JISP16$_{2010}$ *NN* interaction.

Partial wave	$^{1}s_0$	$^{3}p_0$	$^{1}p_1$	$^{3}p_1$	$^{3}s_1$–$^{3}d_1$	$^{1}d_2$	$^{3}d_2$	$^{3}p_2$–$^{3}f_2$	$^{3}d_3$–$^{3}g_3$
ϑ	−0.0966°	−8.72°	−15.62°	−6.01°	−11.00°	−2.73°	7.25°	7.00°	0.457°

Table 8. NCFC predictions of the ^{6}Li ground state E_{gs} and excitation E_x energies (in MeV) in comparison with Green's function Monte Carlo (GFMC) results obtained with Argonne AV18 *NN* and Urbana UIX and Illinois IL2 *NNN* interactions. We present in parentheses the estimate of the accuracy of extrapolations A and B of the absolute energies of excited states. For the ground state rms point-proton radius r_p and quadrupole moment Q, we present the interval of values (in fm and $e \cdot \mathrm{fm}^2$, respectively) obtained in the largest model spaces with bare interactions with $\hbar\Omega$ = 15−25 MeV, i. e. in the same interval of $\hbar\Omega$ values that was used in extrapolation A for the ground state.

	JISP16		JISP16$_{2010}$		AV18+UIX	AV18+IL2	
	Extrap. A	Extrap. B	Extrap. A	Extrap. B	GFMC [8,35]	GFMC [9,35]	
$E(J^\pi, T)$	$N_{\max}$ = 10−16	$N_{\max}$ = 12−16	$N_{\max}$ = 8−14	$N_{\max}$ = 10−14			Experim.
$E_{gs}(1^+, 0)_1$	−31.47(0.09)	−31.48(0.03)	-31.33(0.16)	-31.34(0.07)	−31.25(8)	−32.0(1)	−31.994
r_p	2.137–2.240		2.109–2.225		2.46(2)	2.39(1)	2.32(3)
Q	−0.071– −0.075		−0.081– −0.102		−0.33(18)	−0.32(6)	−0.082(2)
$E_x(3^+, 0)$	2.56(0.04)	2.55(0.07)	2.08(0.16)	2.097(0.003)	2.8(1)	2.2	2.186
$E_x(0^+, 1)$	3.68(0.06)	3.65(0.06)	3.46(0.18)	3.498(0.007)	3.94(23)	3.4	3.563
$E_x(2^+, 0)$	4.5(0.1)	4.5(0.2)	4.5(0.3)	4.39(0.16)	4.0(1)	4.2	4.312
$E_x(2^+, 1)$	5.9(0.1)	5.9(0.1)	5.8(0.3)	5.72(0.05)		5.5	5.366
$E_x(1^+, 0)_2$	5.4(0.3)	5.4(0.2)	5.5(0.7)	5.72(0.25)	5.1(1)	5.6	5.65

act binding energies of nuclei with $10 \le A \le 16$ and only slightly underbinds some of lighter nuclei listed in Table 6.

Table 8 presents the results of ^{6}Li properties calculations with JISP16 and JISP16$_{2010}$. It is seen that JISP16 and JISP16$_{2010}$ provide more or less the same quality of ^{6}Li properties: the binding energy is better described by JISP16 but the excitation spectrum is are better described by JISP16$_{2010}$. Both JISP16 and JISP16$_{2010}$ describe ^{6}Li with a quality similar to the Argonne AV18 *NN* interaction in combination with Urbana UIX *NNN* force. Both JISP16 and JISP16$_{2010}$ also provide a comparable description of ^{6}Li as AV18 in combination with Illinois IL2 *NNN* interaction: AV18+IL2 is more accurate for the binding energy prediction, overestimates the rms point-proton radius by approximately the same value as the underestimation of r_p by JISP16 and JISP16$_{2010}$ interactions (note however that the r_p value is not completely converged in our calculations and still increases with $N_{\max}$), provides more or less the same accuracy for excitation energies, but the ^{6}Li quadrupole moment calculated with AV18+IL2 is significantly larger than the experiment.

We plan to explore the properties of the refined realistic nonlocal *NN* interaction JISP16$_{2010}$ in systematic large-scale calculations of other light nuclei including the ones with $A > 16$ and away from $N \sim Z$, and to carefully study its predictions not only for the binding energies but also for the spectra, electromagnetic transitions and other observables. Our plan is also to tune the interaction to the description of nuclear matter properties.

5 Concluding remarks

We believe that JISP16$_{2010}$ has good prospects to success in the nuclear structure studies. This *NN* interaction provides a high-quality description of the *NN* data together with a very reasonable description of many-body nuclear systems without referring to *NNN* forces. Moreover, a very

specific form of this interaction — small-rank matrix in the oscillator basis with a reasonable $\hbar\Omega$ value — is responsible for a fast convergence of shell model calculations which makes it possible to rely on bare interaction results and extrapolate them to infinite model space. We consider this *NN* interaction as an important realistic ingredient of the new accurate *ab initio* NCFC approach in nuclear structure theory.

In constructing JISP-type *NN* interaction models, we adopted only the accepted symmetries of the strong interaction and neglected explicit constraints such as the long-range behavior from meson-exchange theory. However, this does not mean that the JISP16 and JISP16$_{2010}$ interactions are inconsistent with meson-theoretical forms of the *NN* interaction. On the contrary, it is well-known that the one-pion exchange dominates the *NN* interaction in higher partial waves and the long-range behavior of *NN* interaction in lower partial waves. In this context, we showed in Ref. [18] that our scattering wave functions in higher partial waves are nearly indistinguishable from those of the Nijmegen-II meson-exchange potential. Also, in lower partial waves, our wave functions are very close to those of Nijmegen-II at large distances and a small difference is seen only at higher energies. Finally, we introduced the PETs of JISP16 and JISP16$_{2010}$ only in lower partial waves and only in a few lowest oscillator components of the potential with a large value of $\hbar\Omega = 40$ MeV. As a result, PETs reshape the wave functions at short distances ($\lesssim 1$ fm) only. Thus, the JISP-type interactions appear to be consistent with the well-established pion-exchange tail as embodied in the Nijmegen-II *NN* interaction.

We propose our JISP16$_{2010}$ as a realistic *NN* interaction describing the two-body observables with high precision and providing a reasonable economic description of properties of many-body nuclear systems in microscopic *ab initio* approaches. The economy arises from the softness of the interaction represented in a separable oscillator form. Short distance phase-equivalent transformations adjust the off-shell properties successfully to reduce the roles of multi-nucleon interactions. The particular mechanism of this reduction is still not completely clear. However, our results clearly demonstrate that such a mechanism exists and should be studied in detail.

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