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INVERSE SCATTERING *NN* INTERACTION JISP AND *AB INITIO* THEORY OF LIGHT NUCLEI

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We discuss the studies of light nuclei in *ab initio* No-core Full Configuration approach based on extrapolations to the infinite model space of large-scale No-core Shell Model calculations on supercomputers. The convergence at the end of *p* shell and beginning of the *sd* shell can be achieved if only reasonable soft enough *NN* interactions are used. In particular, good predictions are obtained with a realistic JISP16 *NN* interaction obtained in *J*-matrix inverse scattering approach and fitted to reproduce light nuclei observables without three-nucleon forces. We discuss the current status of this *NN* interaction and its recent development.

Мы обсуждаем исследование легких ядер в подходе *ab initio* No-core full configuration, основанном на экстраполяции на бесконечное модельное пространство расчетов в модели оболочек без инерного кора с использованием больших базисов, проводимых на суперкомпьютерах. Сходимость для ядер в конце *p*-оболочки и начале *sd*-оболочки может быть достигнута только при использовании достаточно мягкого *NN*-взаимодействия. В частности, хорошие предсказания получаются с реалистическим *NN*-взаимодействием JISP16, полученным методом обратной задачи рассеяния и подогнанным для воспроизведения наблюдаемых в легких ядрах без использования трехчастичных сил. Мы обсуждаем текущий статус этого *NN*-взаимодействия и его развитие в последнее время.

Keywords: realistic nucleon-nucleon interaction, the shell model without an inert core, the spectra of light nuclei, the formalism of J-matrix method.

INTRODUCTION

One of the mainstreams of modern nuclear theory is an *ab initio* description of nuclei, i. e. model-free calculations of many-nucleon systems using supercomputers. A rapid development of *ab initio* methods for solving finite nuclei has opened a range of nuclear phenomena that can be evaluated to high precision using realistic nucleon-nucleon interactions. 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. Recently a new *ab initio* method, the No-core Full Configuration (NCFC) approach [4], was introduced. NCFC is based on extrapolation of the NCSM results 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 concentrate the discussion here on the NCFC approach and on some new results obtained with it. In particular, we discuss the predictions [5] for the binding energy and spectrum of the extreme proton-excess nucleus ^{14}F confirmed by the first experimental observation of this isotope reported recently [6].

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 [7], Nijmegen [8], Argonne [9]) have been developed that should be used together with modern *NNN* forces (Urbana [10, 11], Illinois [12], Tucson–Melbourne [13–15]) to reproduce properties of many-body nuclear systems. On the other hand, one sees the emergence of realistic *NN* and *NNN* interactions with ties to QCD [16–19].

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) [20, 21] and JISP (*J*-matrix Inverse Scattering Potential) [22–25] 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 [26] who demonstrated 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.

The JISP *NN* interaction provides a fast convergence of NCSM calculations, it is fitted in NCSM and NCFC studies to the properties of light nuclei and is developing together with the progress in these *ab initio* approaches. We discuss here the progress in developing of the JISP *NN* interaction in line with related progress of NCSM and NCFC studies of light nuclei.

JISP16 *NN* INTERACTION AND NCFC APPROACH

The *J*-matrix inverse scattering approach was suggested in Ref. [27]. It was further developed and used to design a high-quality JISP *NN* interaction in Ref. [22]. A nonlocal interaction obtained in this approach is in the form of a matrix in the oscillator basis in each of *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 the 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 [22], i. e., the JISP *NN* interaction matrices include all relative *NN* motion oscillator states with excitation quanta $N_{\max}$ up to 8 or 9 depending on parity. In other words, we use potential matrices of the rank $r = 5$ in s and p 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 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) [28].

PETs originating from unitary transformations of the oscillator basis proposed in Refs. [29, 30], give rise to ambiguity of the interaction obtained in the *J*-matrix inverse scattering approach. This ambiguity is 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 [22]. 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. It is worth noting here that the deuteron binding energy E_d and asymptotic normalization constants 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 in Refs. [23, 24]. 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 *NN* interaction [25, 31] fitted to nuclei with masses up through $A \leq 16$.

The JISP16 *NN* interaction provides a good description of binding energies, spectra and other properties of *s* and *p* shell nuclei. It was used in a number of pa-

pers of various groups [4, 5, 25, 32–44] and was shown to be one of the best if not the best as compared to other modern models of the realistic strong interaction from the point of view of description of observables in light nuclei. It is worth noting that JISP16 provides better convergence of *ab initio* calculations than other realistic *NN* interactions and avoids the need to use three-nucleon forces. As a result, the JISP16 predictions for light nuclei are more reliable than that of other realistic models of *NN* interactions. With modern supercomputer facilities, we can obtain converged or nearly converged energies of nuclei with mass $A \leq 6$. For calculations of heavier nuclear systems, we proposed recently a NCFC approach [4].

It was found [4] that binding energies of many light nuclei represent an exponential convergence pattern in the excitation oscillator quanta $N_{\max}$ characterizing the basis space of the NCSM. Therefore, we fit the set of ground state energies obtained with each fixed $\hbar\Omega$ value using the relation

$$E_{gs}(N_{max})=\alpha\exp(-cN_{max})+E_{gs}(\infty) \quad (1)$$

where fitting parameters *a* and *c* depend on the $\hbar\Omega$ value and $E_{gs}(\infty)$ is the extrapolated ground state energy in the infinite basis space. The exponential convergence patterns and fits by Eq. (1) are illustrated by Fig. 1. Within the NCFC approach, 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 [4].

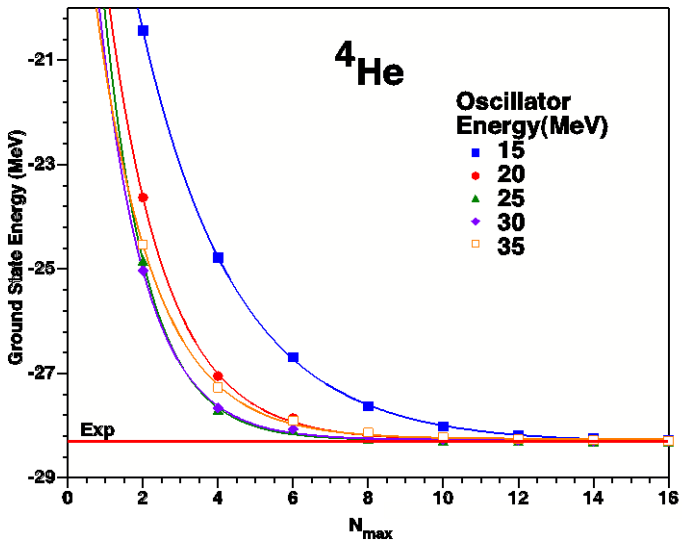

Fig. 1. Ground state energies of ^{4}He obtained with different $N_{\max}$ and $\hbar\Omega$ values. Each set of points at fixed $\hbar\Omega$ is fitted by Eq. (1) (solid curves). Horizontal line shows the experimental binding energy

An exciting recent result obtained with JISP16 *NN* interaction and NCFC method, is an *ab initio* prediction [5] of properties of the exotic extreme proton-excess nucleus ^{14}F. The first experimental results regarding this isotope became available recently from Cyclotron Institute at Texas A&M University [6]. 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 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 30 504 quad-core compute nodes at the Jaguar supercomputer at ORNL.

We present in Table 1 the results of NCFC calculations [5] of the ^{14}F ground state energy. Combining the extrapolations A and B predictions suggests a binding energy of 72 ± 4 MeV for ^{14}F nicely confirmed by a later experiment [6] where a value of 74.00 MeV was reported. We performed similar calculations for the mirror nucleus ^{14}B with a known binding energy of 85.423 MeV [45]. This value agrees with our prediction from combination of extrapolations A and B 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 [45].

Table 1

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 [5]. Estimates of the accuracy of the extrapolations are shown in parentheses. Experimental data for ^{13}O and ^{14}B are taken from Ref. [45] and from Ref. [6] for ^{14}F.

Nucleus	Extrapolation A	Extrapolation 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)	–74.00

We note that a good description of both ^{14}F and ^{13}O in the same approach is important to ensure consistency of the theory and experiment in which ^{14}F was produced in the $^{13}O + p$ reaction. In this respect it is interesting to note that although the 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. The numerical uncertainty in these differences is unclear, but expected to be significantly smaller than the uncertainty in the total energies.

In calculations of the ^{14}F excitation spectrum [5], we performed independent separate extrapolation fits for total energies of all states. The differences between the extrapolated total energies and the ground state energy is our prediction for the excitation energies. This approach was carefully tested in Ref. [5] in calculations of

the ^{6}Li spectrum where a good convergence can be achieved. Evaluated uncertainties of extrapolated total energies of excited states are of the same order as that of the ground state; nevertheless, as discussed above, we expect the uncertainties of energy differences, i. e., of excitation energies, to be significantly smaller. The obtained spectrum is rather dense and includes many states, however, we expect the five lowest excited states only to have small enough widths (see Ref. [5] for a detailed discussion).

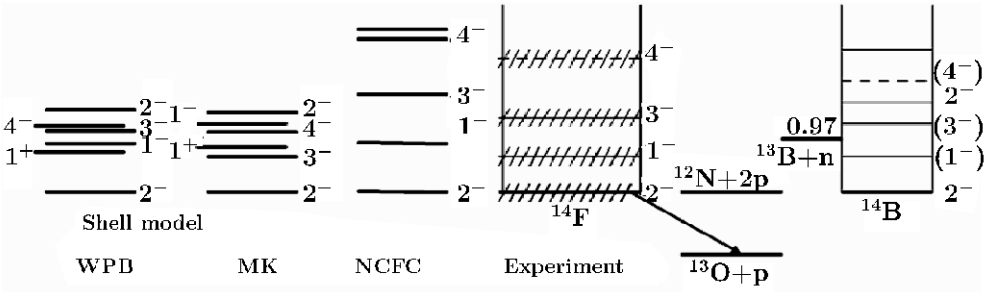

Fig. 2. The ^{14}F spectrum: shell model calculations with WPB and MK interactions [6] and our predictions [5] (NCFC) in comparison with experimental data reported in Ref. [6] (experiment) and that of the mirror ^{14}B nucleus [45]

Several excited states in ^{14}F were observed experimentally [6]. They are compared with our predictions [5] in Fig. 2. The experiment [6] is seen to confirm our predictions for the ^{14}F spectrum [5] obtained before the first observation of this nucleus. These results provide a strong support to our *ab initio* approach based on NCSM calculations, NCFC extrapolations and the use of realistic JISP16 *NN* interaction. The *ab initio* results are seen from Fig. 2 to reproduce the experiment much better than conventional shell model calculations with an inert core and phenomenological effective interactions WPB and MK.

We present here spectra of excited states of several nuclei calculated in the NCFC approach. They are compared with ones observed experimentally in Fig. 3. We have chosen only narrow states with width less then 300 keV with minimal isospin for a given nucleus. However, in case of ^{7}Li we show both $5/2^{-}$ excited states though the width of one of them is 880 keV. On the other hand, in case of ^{10}B we obtained in calculations only two 1^{+} states while there are three such states known experimentally. It is seen that in most cases the calculated with JISP16 interaction excited levels lie slightly above the experimental ones. The ordering of theoretical levels is correct in most cases.

We note that the NCFC calculation of some states can be a complicated non-trivial problem. We illustrate this by calculation of the first and second excited states in ^{10}B. These states are known experimentally to be 1^{+} states, the ground state in ^{10}B is a 3^{+} state. It is conventionally believed that the spin of the ^{10}B ground state cannot be reproduced without *NNN* forces.

However, a purely two-nucleon interaction JISP16 is able to reproduce correctly the ground state spin in ^{10}B, but this requires an accurate treatment of 1^+ states.

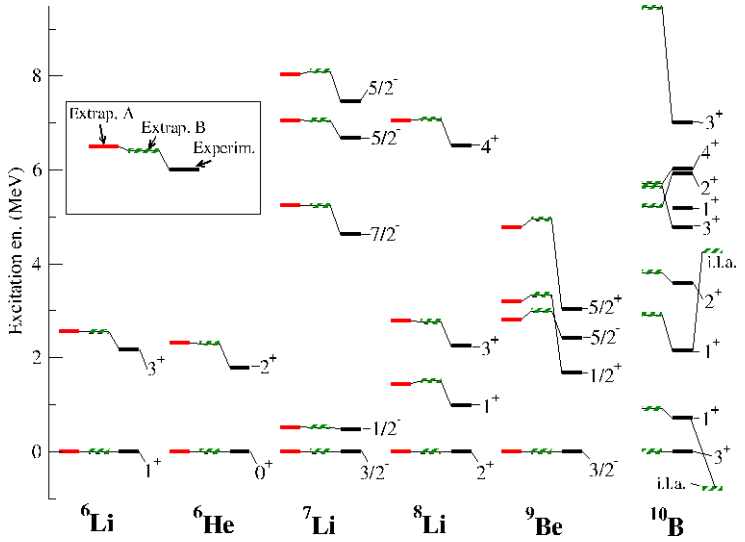

Fig. 3. Energy spectra of few *p* shell nuclei obtained with JISP16. i.l.a. means initial level assignment (see text for details)

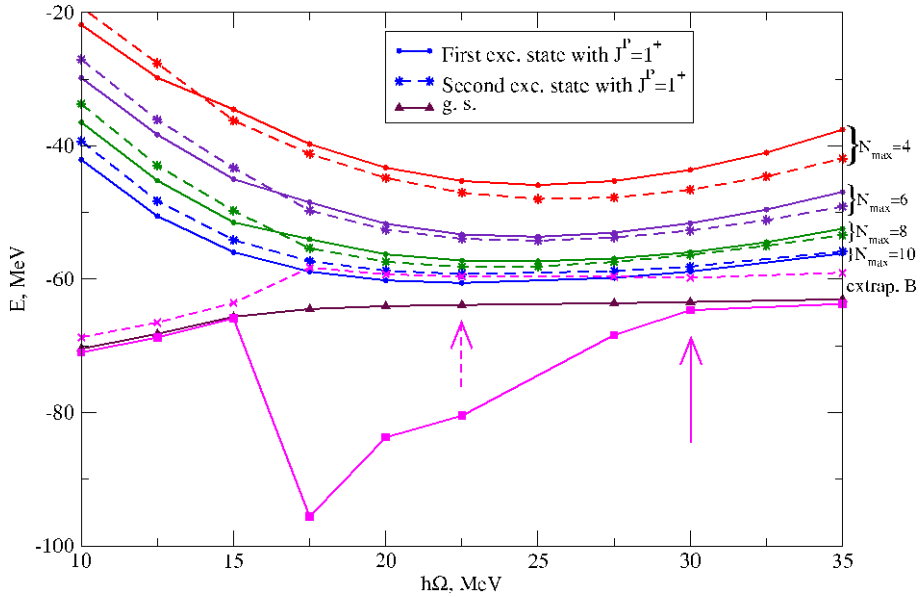

Fig. 4. NCSM calculations and extrapolation B results for first two 1^+ states in ^{10}B with the level assignment based on dynamics of the occupation probabilities of lowest single-particle states (initial level assignment). Arrows indicate the most reliable $\hbar\Omega$ values for the extrapolation B

These 1^+ states are very close in energy and in the NCSM calculations we see the crossing of these states as functions of $\hbar\Omega$ (see Fig. 4). For the NCSM extrapolation we need to pick up a given state with this or that $\hbar\Omega$ value for a set of results obtained with different $N_{\max}$ values. Therefore we need a careful assignment for each state. State assignment shown in Fig. 4 was performed according to the dynamics of the occupation probabilities of lowest single-particle states. As a result, the NCSM extrapolated energies demonstrate a non-monotonic behavior with pronounced jumps (see Fig. 4).

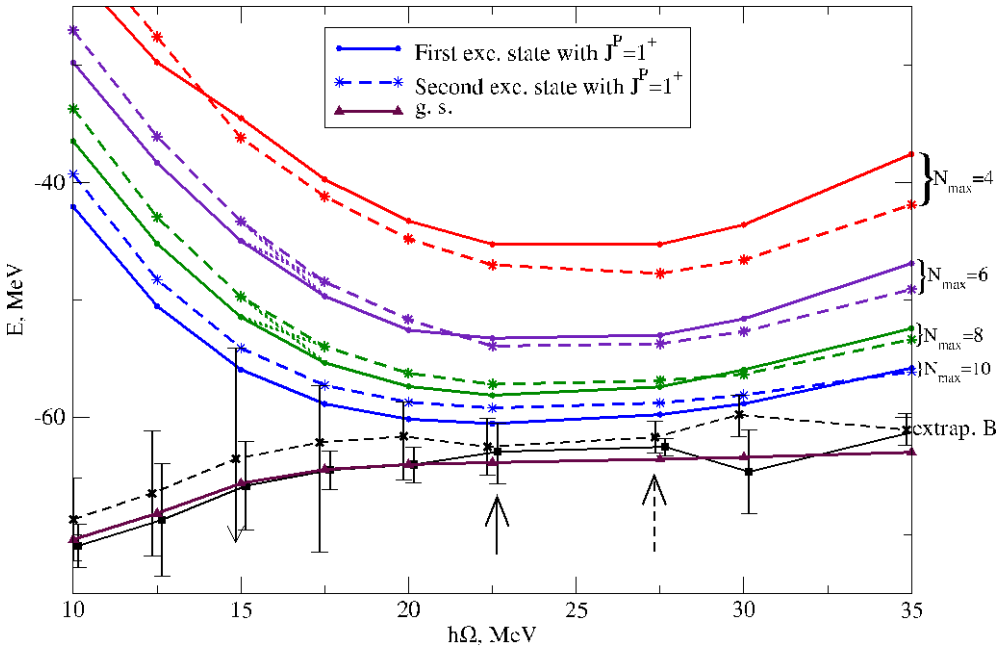

Fig. 5. The same as Fig. 4 but for the 1^+ level assignment based on rms radii and quadrupole moments (alternative level assignment)

In Fig. 5 we show an alternative level assignment of these states based on rms radii and quadrupole moments of these states. With this prescription, the level crossings for $N_{\max} = 6$ and 8 shift to higher $\hbar\Omega$ values (dotted lines in Fig. 5 demonstrate the crossings obtained with the initial level assignment of Fig. 4). As a result, the behavior of the NCSM extrapolated energies of these states become smother and more stable. The non-smooth behavior is seen only around $\hbar\Omega = 30$ MeV. Note, the $N_{\max} = 8$ results obtained with $\hbar\Omega = 30$ MeV for these levels are very close in energy and the levels are essentially mixed in this case. The most reliable $\hbar\Omega$ values for the extrapolation B (shown by arrows in Fig. 5) should be picked up from the interval of flat $\hbar\Omega$ -dependence of extrapolated energies.

In Fig. 3 we present the ^{10}B results obtained with 1^+ level assignment of Fig. 5; the position of 1^+ states obtained with the initial level assignment of Fig. 4 are labeled with i.l.a. in Fig. 3. It is seen that the inaccurate initial 1^+ level assignment results in incorrect spin of the ^{10}B ground state. However, with the more accurate 1^+ level assignment we obtain the ^{10}B ground state with the correct spin. The spectrum of ^{10}B is reasonably well reproduced in the NCFC approach with JISP16 *NN* interaction.

REFINED JISP16$_{2010}$ INTERACTION

The new NCFC approach provides much more reliable *ab initio* predictions for bindings than an earlier pure NCSM approach. The NCFC extrapolation technique revealed some drawbacks of the JISP16 *NN* interaction that was fitted to nuclear observables before this technique was developed. In particular, it was found that the JISP16 interaction overbinds essentially nuclei with mass $A>=14$ and $N\approx Z$.

These deficiencies of the *NN* interaction can be addressed by a new fit in the NCFC calculations of the PET parameters defining JISP interaction. We refer to as JISP16$_{2010}$ the revised *NN* interaction obtained in this fit. The JISP16 and JISP16$_{2010}$ describe *NN* scattering data with the same accuracy; the same PET defines both these interactions in the *sd* partial wave, hence they predict the same deuteron properties. However PET parameters in other *NN* partial waves differ between JISP16$_{2010}$ and JISP16. We note also that JISP16 was defined only in the *NN* partial waves with momenta $J<=4$ while the JISP16$_{2010}$ is extended to all $J<=8$.

We compare binding energies of some nuclei obtained with JISP16 and JISP16$_{2010}$ interactions in Table 2. It is seen that the new interaction essentially improves the description of the *p* shell nuclei. In particular, JISP16$_{2010}$ provides nearly exact binding energies of nuclei with $10<=A<=16$ and only slightly underbinds some of lighter nuclei listed in Table 2.

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 phenomenological nuclear matter properties.

Table 2

Binding energies (in MeV) of some nuclei obtained with JISP16 and JISP16$_{2010}$ *NN* interactions in the NCFC approach and uncertainties of extrapolations; the $N_{\max}$ columns show the largest NCSM basis 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±0.001	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

Table continued…

^{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

An additional possibility for further improvement of the JISP-type *NN* interaction provides DET-PET, a new type of phase-equivalent transformations suggested recently [46, 47]. Contrary to conventional PETs resulting in modification of bound state and scattering wave functions, DET-PET guarantees that the transformed interaction generates not only the same scattering phase shifts and two-body binding energy (or, more generally, bound state energies) but also the same bound state (deuteron) wave function as the initial untransformed interaction. Clearly, DET-PET has the advantage of preserving the deuteron ground-state observables. The DET-PET theory can be easily reformulated to preserve scattering wave functions at a given energy instead of the bound state wave function. On the other hand, DET-PET, as well as any PET, modifies a two-body interaction off-shell, and hence manifests itself in many-body systems. It would be interesting to utilize DET-PET preserving *NN* correlations of the initial realistic *NN* interaction in modifications of this interaction aimed to fit the description of light nuclei.

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