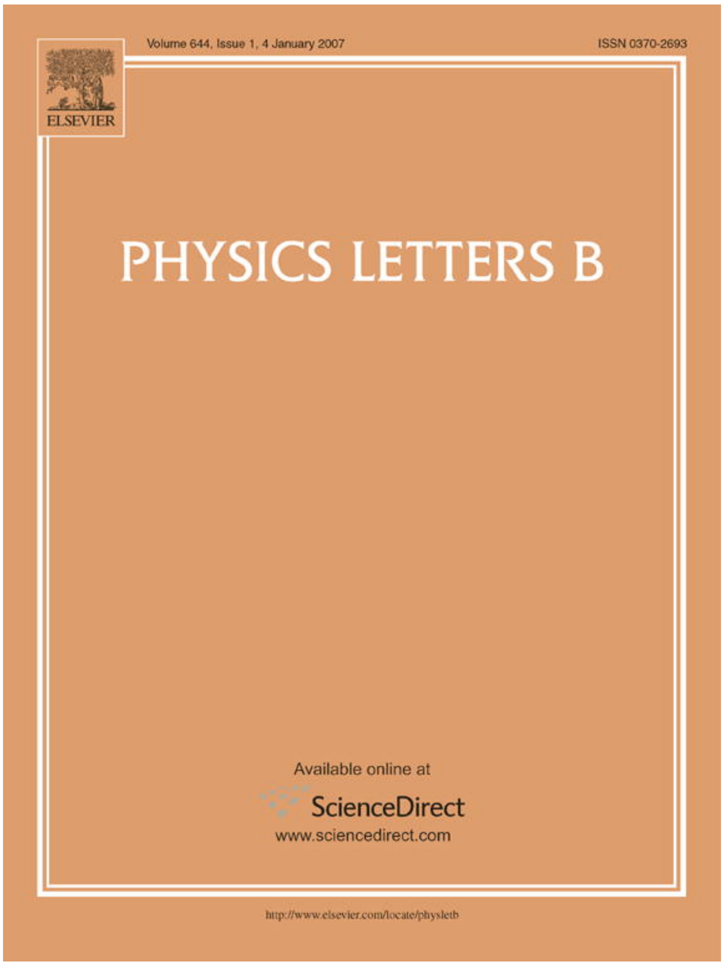
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Realistic nuclear Hamiltonian: Ab exitu approach

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Abstract

Fully-microscopic no-core shell model (NCSM) calculations of all stable s and p shell nuclei are used to determine a realistic NN interaction, JISP16, describing not only the two-nucleon data but the binding energies and spectra of nuclei with $A \leqslant 16$ as well. The JISP16 interaction, providing rapid convergence of the NCSM calculations, is obtained in an ab exitu approach by phase-equivalent transformations of the JISP6 NN interaction.

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To complement the successful but computationally intensive 'ab initio' no-core shell model (NCSM) [1], we introduce the 'ab exitu' NCSM. While the former has proven very successful for light nuclei when one includes three-body (NNN) forces [2,3], the computational complexity motivates us to introduce an approach that simultaneously minimizes NNN forces while providing more rapid convergence with a pure nucleon–nucleon (NN) force. We invoke directly an end-goal of nuclear theory (hence the term 'ab exitu'), a successful description of nuclear properties, including the available NN data, to develop a new class of NN potentials that provide accurate descriptions of a broad range of nuclear data.

To achieve this, we form a union of two recent techniques—the J-matrix inverse scattering [4–6] and the NCSM [1]. A major ingredient of our approach is the form of the NN interaction (a small matrix in the oscillator basis), which is chosen to provide rapid convergence of many-body observables within the NCSM. Indeed, we show below that results up through $A = 16$ obtained directly with the bare interaction (one that accurately describes the NN data) are close to those obtained with the effective interaction and are very useful to establish the confidence region for the binding energy.

Since this is a departure from the more traditional approach, we motivate our development with observations concerning the successful ab initio approaches to light nuclei. Indeed several promising microscopic approaches have been introduced and tested extensively with realistic NN interactions (see [7] and references therein) and with realistic $NN + NNN$ interactions [2,3,8]. Progress towards heavier nuclei appears limited only by scientific manpower and by available computers. However, all approaches face the exponentially rising computational complexity inherent in the quantum many-body problem with increasing particle number and novel schemes are needed to minimize the computational burden without sacrificing realism and precision.

The earliest and most successful in reaching nuclei beyond $A = 4$ is the Green's-function Monte Carlo (GFMC) approach [8] whose power has been used to determine a sequence of

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Table 1
JISP16 non-zero matrix elements in $\hbar\omega = 40$ MeV units in the uncoupled NN partial waves that differ from the respective JISP6 matrix elements and of the JISP16 matrices in higher partial waves

n	V^l_{nn}	$V^l_{n,n+1} = V^l_{n+1,n}$	$V^l_{n,n+2} = V^l_{n+2,n}$
$^1p_1$ partial wave			
0	0.4864373541	−0.2359869829	0.3117643519
1	−0.1487460250	−0.1438603014	
$^1g_4$ partial wave			
0	−0.0159359974	0.0110169386	
1	−0.0229351778	0.0073206473	
2	−0.0056121168		
$^3p_0$ partial wave			
0	0.1571004930	−0.1425039101	0.2505691390
1	−0.2172768679	−0.0981725471	
$^3g_4$ partial wave			
0	−0.0762338541	0.0498484441	
1	−0.1107702854	0.0371277135	
2	−0.0295683403		

Table 2
Same as in Table 1 but for the coupled NN waves

sd coupled waves

$V^{ss}_{nn'}$ matrix elements

n	V^{ss}_{nn}	$V^{ss}_{n,n+1} = V^{ss}_{n+1,n}$
0	−0.5125432769	0.2139078754

$V^{dd}_{nn'}$ matrix elements

n	V^{dd}_{nn}	$V^{dd}_{n,n+1} = V^{dd}_{n+1,n}$
0	0.0551475852	−0.0952367414

$V^{sd}_{nn'} = V^{ds}_{n'n}$ matrix elements

n	$V^{sd}_{n,n-1} = V^{ds}_{n-1,n}$	$V^{sd}_{nn} = V^{ds}_{nn}$	$V^{sd}_{n,n+1} = V^{ds}_{n+1,n}$
0		−0.4035852241	0.2003382771
1	−0.0464306332		

pf coupled waves

$V^{pp}_{nn'}$ matrix elements

n	V^{pp}_{nn}	$V^{pp}_{n,n+1} = V^{pp}_{n+1,n}$	$V^{pp}_{n,n+2} = V^{pp}_{n+2,n}$
0	−0.1933759934	0.1508436490	−0.1072949881
1	−0.0277262441	0.0964883300	

$V^{pf}_{nn'}$ matrix elements

n	$V^{pf}_{n,n-1} = V^{fp}_{n-1,n}$	$V^{pf}_{nn} = V^{fp}_{nn}$	$V^{pf}_{n,n+1} = V^{fp}_{n+1,n}$
0		0.0195093232	0.0020663826
1	−0.0252003957	0.0236188613	

dg coupled waves

$V^{dd}_{nn'}$ matrix elements

n	V^{dd}_{nn}	$V^{dd}_{n,n+1} = V^{dd}_{n+1,n}$
0	−0.0226611102	0.0231171026
1	−0.0514940563	0.0256493733
2	−0.0329967376	0.0061799968
3	−0.0002368252	

$V^{gg}_{nn'}$ matrix elements

n	V^{gg}_{nn}	$V^{gg}_{n,n+1} = V^{gg}_{n+1,n}$
0	0.0435654902	−0.0276372780
1	0.0537629744	−0.0140723375
2	0.0079901608	

$V^{dg}_{nn'}$ matrix elements

n	$V^{dg}_{n,n-1} = V^{gd}_{n-1,n}$	$V^{dg}_{nn} = V^{gd}_{nn}$
0		−0.0392683838
1	0.0791431969	−0.0874578184
2	0.0660805779	−0.0334474774
3	0.0029846726	

ever-improving NNN interactions [8–10], in conjunction with highly precise NN interactions [11] that fit a wide selection of low-lying properties of light nuclei up through $A = 10$. In addition, the Hamiltonians are tested for their predictions in infinite systems [12]. According to our usage of terminology here, the application of GFMC to determine successful NNN interactions is an excellent example of an ab exitu approach.

Now, we ask the question whether it is possible to go even further and search through the residual freedoms of a realistic NN interaction to obtain new NN interactions that satisfy three criteria: (1) retain excellent descriptions of the NN data; (2) provide good fits to light nuclei; and (3) provide improved convergence properties within the NCSM. The challenge to satisfy this triad of conditions is daunting and we are able to provide only an initial demonstration at the present time.

We are supported by the work of Polyzou and Glöckle who demonstrated [13] that a realistic NN interaction is equivalent at the $A = 3$ level to a realistic $NN + NNN$ interaction where the new NN force is related to the initial one through a phase-equivalent transformation (PET). The net consequence is that properties of nuclei beyond $A = 3$ become dependent on the freedom within the transformations at the $A = 3$ level. It seems reasonable then to exploit this freedom and work to minimize the need for the explicit introduction of three and higher body forces. However, we do not surmise that we would be able to eliminate them completely.

We start from the realistic charge-independent NN interaction JISP6 [6] that provides an excellent description of the deuteron properties [6] and 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) [14]. JISP6 provides also a very good description of the spectra of p shell nuclei, but we find that it overbinds nuclei with $A \geqslant 10$. To eliminate this deficiency, we exploited PETs to modify the JISP6 in various partial waves. The resulting interaction, hereafter referred to as JISP16 since it is fitted in our ab exitu approach to the spectra and bindings of stable $A \leqslant 16$ nuclei, can be obtained from the initial ISTP interaction in the same manner as JISP6 in Ref. [6] but with a different set of PET angles. These angles associated with unitary transformations (see Refs. [5,6] for details) mixing the lowest s and d oscillator basis states in the coupled sd waves and the lowest oscillator basis states in the $^3p_2$, $^3p_1$, $^3p_0$, $^3d_2$ and $^1p_1$ waves are $\vartheta = -11.0°$, $+5°$, $-6°$, $-10°$, $+25°$ and $-12°$, respectively. The JISP16 matrix elements in the oscillator basis with $\hbar\omega = 40$ MeV that differ from those of JISP6, are presented in Tables 1 and 2. The

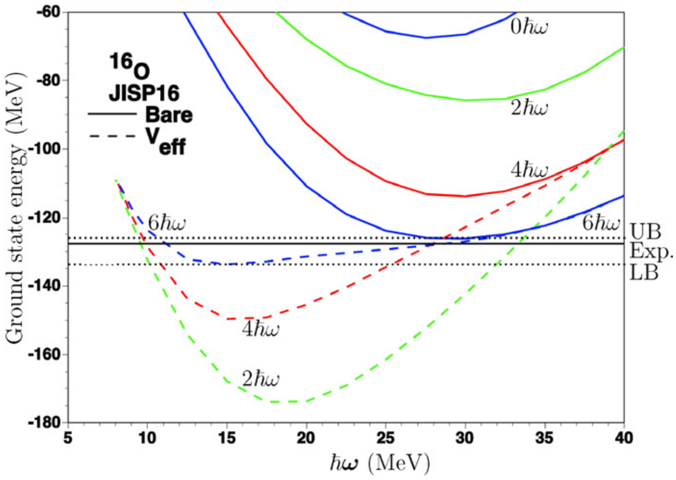

Fig. 1. (Color online.) The $\hbar\omega$ dependence of the ^{16}O ground state energy obtained with bare JISP16 and effective interaction based on JISP16 in a sequence of $N_{\max}\hbar\omega$ model spaces up to $N_{\max} = 6$; the lines marked as Exp., UB and LB show the experimental ground state energy, the upper bound and the suggested lower bound for the NCSM ground state energy predictions.

JISP16 predictions for the deuteron rms radius $r_d = 1.9643$ fm and quadrupole moment $Q = 0.288585\ e \cdot \text{fm}^2$ slightly differ from the JISP6 results since the JISP16 and JISP6 PET angle in the sd coupled waves is slightly different ($\vartheta = -11.0°$ versus $-11.3°$). In this Letter, we include all NN partial waves up to $l = 4$ and include in Tables 1 and 2 the added matrix elements.

Our fitting procedure is one of 'trial-and-error' where we worked with only a few partial waves that we deemed important for these nuclei. We fit only the excitation energies of few lowest ^{6}Li levels and the ^{6}Li and ^{16}O binding energies. To save time, we performed the NCSM calculations in small enough model spaces (up to $10\hbar\omega$ for ^{6}Li and up to $4\hbar\omega$ for ^{16}O). After obtaining a reasonable description of these observables, we checked that the binding energies and spectra of all the rest s and p shell nuclei are well-described in small model spaces. The results presented below 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, however it is still very reasonable. In a future effort, we will perform a thorough search through the space of possible PETs that should further improve the description of nuclear properties while retaining the excellent description of the NN data.

We illustrate our approach with the ^{16}O ground state energy in Fig. 1. The variational principle holds for the bare interaction results; hence the upper bound (UB) for the ground state energy is the minimum of its $\hbar\omega$ dependence in the $6\hbar\omega$ model space. In the calculations with the effective interaction obtained by the Lee–Suzuki transformation, the quoted result is conventionally associated with the minimum of the $\hbar\omega$ dependence. This minimum is seen from Fig. 1 to ascend with increasing model space. Based on our results in lighter systems with larger spaces that show uniform convergence of this minimum, the minimum obtained in the $6\hbar\omega$ model space is a suggested lower bound (LB) for the ground state energy. The difference between these upper and lower bounds is our estimate for the 'error bars' of our predictions. These error bars suggest reasonable convergence is attained but this requires verification in larger basis spaces.

Table 3
Binding energies (in MeV) of nuclei obtained with bare JISP16 and effective interaction generated by JISP16

Nucleus	Nature	Bare	Effective	$\hbar\omega$ (MeV)	Model space
^{3}H	8.482	8.354	8.496(20)	7	$14\hbar\omega$
^{3}He	7.718	7.648	7.797(17)	7	$14\hbar\omega$
^{4}He	28.296	28.297	28.374(57)	10	$14\hbar\omega$
^{6}He	29.269		28.32(28)	17.5	$12\hbar\omega$
^{6}Li	31.995		31.00(31)	17.5	$12\hbar\omega$
^{7}Li	39.245		37.59(30)	17.5	$10\hbar\omega$
^{7}Be	37.600		35.91(29)	17	$10\hbar\omega$
^{8}Be	56.500		53.40(10)	15	$8\hbar\omega$
^{9}Be	58.165	53.54	54.63(26)	16	$8\hbar\omega$
^{9}B	56.314	51.31	52.53(20)	16	$8\hbar\omega$
^{10}Be	64.977	60.55	61.39(20)	19	$8\hbar\omega$
^{10}B	64.751	60.39	60.95(20)	20	$8\hbar\omega$
^{10}C	60.321	55.26	56.36(67)	17	$8\hbar\omega$
^{11}B	76.205	69.2	73.0(31)	17	$6\hbar\omega$
^{11}C	73.440	66.1	70.1(32)	17	$6\hbar\omega$
^{12}B	79.575	71.2	75.9(48)	15	$6\hbar\omega$
^{12}C	92.162	87.4	91.0(49)	17.5	$6\hbar\omega$
^{12}N	74.041	64.5	70.2(48)	15	$6\hbar\omega$
^{13}B	84.453	73.5	82.1(67)	15	$6\hbar\omega$
^{13}C	97.108	93.2	96.4(59)	19	$6\hbar\omega$
^{13}N	94.105	89.7	93.1(62)	18	$6\hbar\omega$
^{13}O	75.558	63.0	72.9(62)	14	$6\hbar\omega$
^{14}C	105.285	101.5	106.0(93)	17.5	$6\hbar\omega$
^{14}N	104.659	103.8	106.8(77)	20	$6\hbar\omega$
^{14}O	98.733	93.7	99.1(92)	16	$6\hbar\omega$
^{15}N	115.492	114.4	119.5(126)	16	$6\hbar\omega$
^{15}O	111.956	110.1	115.8(126)	16	$6\hbar\omega$
^{16}O	127.619	126.2	133.8(158)	15	$6\hbar\omega$

Similar trends are found for most of the p shell nuclei. We present in Table 3 their binding energies obtained with both bare and effective interactions. We also quote the $\hbar\omega$ values providing the minimum with the effective interaction. The difference between the given result and the result obtained with the same $\hbar\omega$ in the next smaller model space is presented in parenthesis to give an estimate of the convergence of our calculations. We quote our differences in significant figures from the rightmost figure of the stated result, omitting decimal points to save space. The ground state energy of $A = 6$, 7 and 8 nuclei converges uniformly from above with both the bare and effective interactions. We present in Table 3 only the effective interaction results for these nuclei due to their superior convergence features. For these nuclei, an extrapolation based on the fit by a constant plus exponential function for different $\hbar\omega$ values may be useful. For ^{6}Li, this extrapolation results in a binding energy of 31.70(17) MeV where the value in parenthesis is the uncertainty of the fit. A similar extrapolation for ^{6}He results in a binding energy of 28.89(17) MeV which is bound with respect to the $\alpha + n + n$ threshold. We note that the bare interaction results for $A = 6$ nuclei are very close to the ef-

Table 4
Ground state energy E_{gs} and excitation energies E_x (in MeV), ground state point-proton rms radius r_p (in fm) and quadrupole moment Q (in $e \cdot \mathrm{fm}^2$) of the ^{6}Li nucleus; $\hbar\omega = 17.5$ MeV

Interaction method	Nature	JISP6 NCSM, $10\hbar\omega$ [6]	JISP16 NCSM, $12\hbar\omega$	AV8' + TM' NCSM, $6\hbar\omega$ [2]	AV18 + UIX GFMC [8,15]	AV18 + IL2 GFMC [10,15]
$E_{gs}(1_1^+, 0)$	−31.995	−31.48	−31.00	−31.04	−31.25(8)	−32.0(1)
r_p	2.32(3)	2.083	2.151	2.054	2.46(2)	2.39(1)
Q	−0.082(2)	−0.194	−0.0646	−0.025	−0.33(18)	−0.32(6)
$E_x(3^+, 0)$	2.186	2.102	2.529	2.471	2.8(1)	2.2
$E_x(0^+, 1)$	3.563	3.348	3.701	3.886	3.94(23)	3.4
$E_x(2^+, 0)$	4.312	4.642	5.001	5.010	4.0(1)	4.2
$E_x(2^+, 1)$	5.366	5.820	6.266	6.482		5.5
$E_x(1_2^+, 0)$	5.65	6.86	6.573	7.621	5.1(1)	5.6

fective interaction ones demonstrating a remarkable softness of the JISP16 interaction: the ^{6}Li and ^{6}He binding energies are 30.94(44) and 28.23(41) MeV, respectively, the extrapolations of the bare interaction bindings produce 31.33(12) MeV for ^{6}Li and 28.61(12) MeV for ^{6}He.

The nuclear Hamiltonian based on the ab exitu realistic NN interaction JISP16, is seen to reproduce well the binding energies of nuclei with $A \leqslant 16$. The lowest state of natural parity has the correct total angular momentum in each nucleus studied. The experimental binding energies of all nuclei presented in Table 3 either lie within error bars of our predictions or are close to our suggested LB based on the effective interaction calculations. Generally JISP16 slightly underbinds only nuclei in the middle of the p shell. The difference between UB and LB is small, suggesting that JISP16 provides good convergence. However, our error bars increase as binding energy decreases in a chain of isobars (cf. the results for ^{13}O and ^{13}N).

We present in Tables 4 and 5 spectra and ground state properties of ^{6}Li and ^{10}B which are known [2,8,15,16] to be sensitive to an explicit NNN interaction. Here, the ab exitu JISP16 NN interaction alone provides a good description. The JISP16 ^{6}Li spectrum seems to be less favorable than that provided by our JISP6 interaction specifically fitted to the ^{6}Li spectrum. However, the JISP16 ^{6}Li spectrum is competitive with those of realistic $NN + NNN$ potential models. Also, we obtain a good description of the ^{6}Li quadrupole moment Q 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. We observe that Q and the point-proton rms radius r_p have a more prominent $\hbar\omega$ dependence than the binding energy.

The ^{10}B properties are also seen to be well-described with the JISP16 interaction contrary to previous results from pure realistic NN interactions [2,16]. We note that the ^{10}B spectrum depends on $\hbar\omega$ at $N_{\max} = 8$ but not so strongly as to alter our main conclusions. For example, the minimum of the ^{10}B ground state corresponds to $\hbar\omega = 20$ MeV while the minimum in the first excited state energy occurs at $\hbar\omega = 15$ MeV. We present in Table 5 the ^{10}B properties obtained with $\hbar\omega = 15$ MeV, i.e. with the $\hbar\omega$ value corresponding to the minimum of the first excited state since it has a more pronounced $\hbar\omega$ dependence than the ground state. The ^{10}B ground state spin was not previously reproduced with a pure realistic NN interaction. We observe that our description of the ^{10}B spectrum is somewhat better than the one obtained with the Argonne AV8' NN potential and Tucson–Melbourne TM' NNN force. In particular, we reproduce the ordering of ^{10}B levels except for the $(3_2^+, 0)$ state. We note that the $(3_2^+, 0)$ state is also too high with the AV8' + TM' interaction.

Table 5
Same as in Table 4 but for the ^{10}B nucleus; $\hbar\omega = 15$ MeV

Interaction method	Nature	JISP16 NCSM, $8\hbar\omega$	AV8' + TM' NCSM, $4\hbar\omega$ [2]	AV18+IL2 GFMC [16]
$E_{gs}(3_1^+, 0)$	−64.751	−60.14	−60.57	−65.6(5)
r_p	2.30(12)	2.168	2.168	2.33(1)
Q	+8.472(56)	6.484	+5.682	+9.5(2)
$E_x(1_1^+, 0)$	0.718	0.555	0.340	0.9
$E_x(0^+, 1)$	1.740	1.202	1.259	
$E_x(1_2^+, 0)$	2.154	2.379	1.216	
$E_x(2_1^+, 0)$	3.587	3.721	2.775	3.9
$E_x(3_2^+, 0)$	4.774	6.162	5.971	
$E_x(2_1^+, 1)$	5.164	5.049	5.182	
$E_x(2_2^+, 0)$	5.92	5.548	3.987	
$E_x(4^+, 0)$	6.025	5.775	5.229	5.6
$E_x(2_2^+, 1)$	7.478	7.776	7.491	

In constructing ISTP [5], JISP6 [6] and JISP16 potentials we adopted only the accepted symmetries of the NN interaction and neglected explicit constraints such as the long-range behavior from meson-exchange theory. However, this does not mean that the JISP16 NN interaction is inconsistent with meson-theoretical forms of the NN interaction. On the contrary, it is well known that the one-pion exchange (OPE) 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. [5] that our scattering wave functions in higher partial waves are nearly indistinguishable from those of the Nijmegen-II OPE 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 JISP6 and JISP16 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). Thus, the JISP16 interaction appears to be consistent with the well-established OPE tail as embodied in the Nijmegen-II NN interaction.

We propose our ab exitu JISP16 as a realistic NN interaction since it describes the two-body observables with high precision. In addition, it provides a reasonable and economic description of properties of many-body nuclear systems in the microscopic NCSM approach. 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 not clear at the present time. However, our results as well as the success of the approach of Ref. [17], clearly demonstrate that such a mechanism exists and should be studied in detail. We plan to study this with explicit NNN interactions.

We conclude that the many-body nuclear Hamiltonian obtained in our ab exitu approach is realistic from the point of view of providing a good description of a wide range of nuclear data. The suggested JISP16 NN interaction opens a path for extending realistic microscopic theory to heavier nuclei, to achieve better convergence and to obtain improved agreement with experiment.

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