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Realistic nuclear Hamiltonian: *Ab exitu* approach

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Fully-microscopic No-core Shell Model (NCSM) calculations of all stable s and p shell nuclei are used to determine realistic NN interaction JISP16 describing not only the two-nucleon data but the binding energies and spectra of nuclei with $A \leq 16$ 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.

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 forces [2, 3], the computational complexity motivates us to introduce an approach that simultaneously minimizes three-body forces while providing more rapid convergence with a pure two-body force. We invoke directly an end-goal of nuclear theory (hence the term '*ab exitu*'), a successful description of the observed properties of nuclei, as well as the available nucleon-nucleon (NN) data, to develop a new class of NN potentials that provide accurate descriptions of a broad range of data accompanied by rapid convergence within the NCSM.

Our approach features a union of two recent techniques — the J-matrix inverse scattering [4–6] and the NCSM, in an iterative scheme that produces new bare NN interactions with high quality descriptions of both NN data and properties of light nuclei. 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 in the NCSM are close to that obtained with the effective interaction and are very useful to establish the confidence region for the binding energy. We show that it is not necessary to sacrifice the quality of the description of the available NN data when fitting, with improved convergence, properties of light nuclei through $A = 16$.

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 the capacity of 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 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 some $NN + NNN$ 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 to carry out the reverse procedure and work to minimize the role of three and higher body forces.

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 $A \geq 10$. To eliminate this deficiency, we exploited PETs to modify the JISP6 in various partial

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TABLE I: 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		

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 $A \leq 16$ 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 I–II. The JISP16 predictions for the deuteron rms radius $r_d = 1.9643$ fm and quadrupole moment $Q = 0.288585$ 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 paper, we extended the NCSM calculations to include all NN partial waves up to $l = 4$; hence we fitted the NN g waves and present in Tables I–II the respective JISP16 matrix elements.

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 our proposed 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 are seen to be quite small and suggest reasonable convergence is attained.

TABLE II: Same as in Table I but for the coupled NN waves.

n			
	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		

Similar trends are found for most of the p shell nuclei. We present in Table III the binding energies of these nuclei obtained with both bare and effective interactions. The $\hbar\omega$ values providing the minimum of the $\hbar\omega$ dependence in calculations with the effective interaction, are

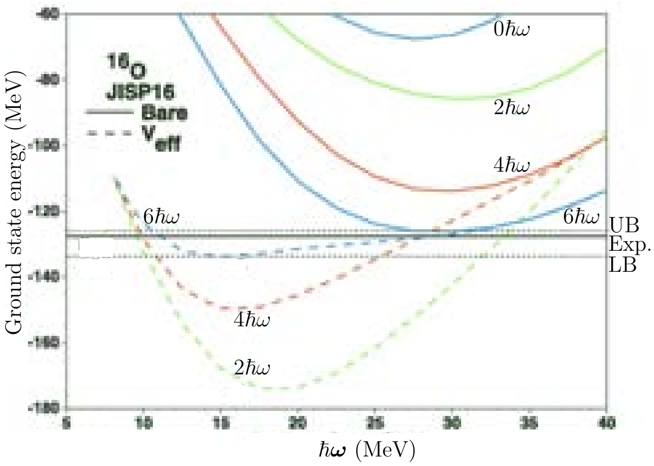

FIG. 1: (Color online) The $\hbar\omega$ dependence of the ^{16}O ground state energy obtained with bare JISP16 and effective interaction based on JISP16 in a sequence of $N_{max}\hbar\omega$ model spaces up to $N_{max} = 6$; the lines marked as Exp., UB and LB show the experimental ground state energy,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

also presented in the Table. The difference between the given result and the result obtained in the next smaller model space is presented in parenthesis to give an estimate of the convergence of our calculations. The ground state energy of $A = 6$ and 7 nuclei converges uniformly from above with both the bare and effective interactions. We present in Table III only the effective interaction results for these nuclei due to their superior convergence features. The lowest state of natural parity has the correct total angular momentum in each nucleus studied.

The nuclear Hamiltonian based on the *ab exitu* realistic NN interaction JISP16, is seen to reproduce well the binding energies of nuclei with $A \leq 16$. The experimental binding energies of most nuclei presented in Table III lie within error bars of our predictions. JISP16 slightly underbinds only nuclei with $A = 8$–11. For ^{6}Li, our extrapolation based on the fit by a constant plus exponential function for different $\hbar\omega$ values 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 effective 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 result in the values of 31.33(12) MeV for ^{6}Li and 28.61(12) MeV for ^{6}He.

We present in Tables IV and V spectra and ground state properties of ^{6}Li and ^{10}B which are known [2, 8, 15, 16] to be sensitive to the presence of the explicit

TABLE III: 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		37.07(25)	15	$6\hbar\omega$
^{7}Be	37.600		35.39(26)	15	$6\hbar\omega$
^{8}Be	56.500	49.58	53.30(3)	15	$6\hbar\omega$
^{9}Be	58.165	50.60	54.91(88)	15	$6\hbar\omega$
^{9}B	56.314	48.28	52.84(88)	15	$6\hbar\omega$
^{10}Be	64.977	57.5	61.9(20)	16	$6\hbar\omega$
^{10}B	64.751	57.4	61.0(18)	17	$6\hbar\omega$
^{10}C	60.321	52.1	57.1(19)	15	$6\hbar\omega$
^{11}B	76.205	63.3	76.1(45)	17	$4\hbar\omega$
^{11}C	73.440	60.1	73.3(45)	17	$4\hbar\omega$
^{12}B	79.575	64.0	80.7(62)	15	$4\hbar\omega$
^{12}C	92.162	81.1	95.8(77)	17.5	$4\hbar\omega$
^{12}N	74.041	57.1	75.0(63)	15	$4\hbar\omega$
^{13}B	84.453	64.2	88.8(78)	15	$4\hbar\omega$
^{13}C	97.108	85.8	102.7(108)	17.5	$4\hbar\omega$
^{13}N	94.105	82.1	99.5(98)	17.5	$4\hbar\omega$
^{13}O	75.558	53.0	79.5(68)	15	$4\hbar\omega$
^{14}C	105.285	92.6	115.3(138)	17.5	$4\hbar\omega$
^{14}N	104.659	95.1	115.6(134)	17.5	$4\hbar\omega$
^{14}O	98.733	84.4	108.2(138)	17.5	$4\hbar\omega$
^{15}N	115.492	104.1	132.0(188)	17.5	$4\hbar\omega$
^{15}O	111.956	99.6	128.1(188)	17.5	$4\hbar\omega$
^{16}O	127.619	126.2	133.8(158)	15	$6\hbar\omega$

three-body force. We see in Tables IV and V that the *ab exitu* JISP16 NN interaction alone provides a good description of ^{6}Li and ^{10}B properties. 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 modern realistic $NN + NNN$ potential models. We note a reasonable JISP16 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. It is worth noting also that the point-proton rms radius r_p and the quadrupole moment Q 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

TABLE IV: 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 $e \cdot \text{fm}^2$) 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

TABLE V: Same as in Table IV but for the ^{10}B nucleus; $\hbar\omega = 16$ MeV.

Interaction Method	Nature	JISP16 $6\hbar\omega$	AV8'+TM' NCSM, $4\hbar\omega$ [2]	AV18+IL2 GFMC [16]
$E_{gs}(3_1^+,0)$	−64.751	−60.96	−60.57	−65.6(5)
r_p	2.30(12)	2.131	2.168	2.33(1)
Q	+8.472(56)	+6.038	+5.682	+9.5(2)
$E_x(1_1^+,0)$	0.718	0.765	0.340	0.9
$E_x(0^+,1)$	1.740	1.176	1.259	
$E_x(1_2^+,0)$	2.154	2.368	1.216	
$E_x(2_1^+,0)$	3.587	3.657	2.775	3.9
$E_x(3_2^+,0)$	4.774	6.310	5.971	
$E_x(2_1^+,1)$	5.164	5.053	5.182	
$E_x(2_2^+,0)$	5.92	5.421	3.987	
$E_x(4^+,0)$	6.025	5.536	5.229	5.6
$E_x(2_2^+,1)$	7.478	8.082	7.491	

from pure realistic two-nucleon interactions [2, 16]. We note that the ^{10}B spectrum depends on $\hbar\omega$ at $N_{max} = 6$ but not so strongly as to alter our main conclusions. For example, the minimum of the ^{10}B ground state corresponds to $\hbar\omega = 17$ MeV while the minimum in the first excited state energy corresponds to $\hbar\omega = 14$ MeV. Therefore, we present in Table V the ^{10}B properties obtained with $\hbar\omega = 16$ MeV which represents a compromise in these minima. The ^{10}B ground state spin was not previously reproduced with a pure realistic two-nucleon 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 predicted to be too high by the AV8' + TM' interaction model.

We conclude that the *ab exitu* Hamiltonian based on the proposed realistic NN JISP16 interaction opens a new perspective for microscopic calculations in nuclear physics. In particular, it provides a possibility to extend realistic microscopic calculations in the NCSM to heavier nuclei and to achieve better convergence while retaining an accurate description of the NN data.

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