Elements of the *ab initio* No Core Shell Model

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Abstract. We outline the *ab initio* no core shell model and present recent results. Nuclear properties are evaluated with two-nucleon (NN) and three-nucleon interactions (TNI) derived within effective field theory (EFT) based on chiral perturbation theory (ChPT). Fitting two available parameters of the TNI generates good descriptions of light nuclei. In another effort, referred to as the *ab exitu* approach, results are obtained with a realistic NN interaction derived by inverse scattering theory with off-shell properties tuned to fit light nuclei. Both approaches produce good results for observables sensitive to spin-orbit properties. In a third approach, we supplement the derived realistic effective interaction with phenomenological NN interaction terms with the goal to describe spectra of fp-shell nuclei in the limited basis spaces currently available.

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INTRODUCTION

Recent advances in microscopic many-body methods have opened new paths for investigating both the strong interaction itself as well as the many facets of nuclear phenomena evident in light nuclei. Once the *ab initio* no core shell model (NCSM) was introduced and shown to be reasonably convergent [1], opportunities emerged for precision testing of the properties of the strong interaction in the nuclear medium. Our focus in this presentation will be on recent and complementary efforts to determine important features of the strong interaction through the resulting properties of nuclei in the p-shell. Selected observables are especially sensitive to the three-nucleon interaction (TNI) and to the off-shell properties of the NN interaction. We also examine the degree to which phenomenological modifications of the NN interactions can improve agreement with experiment, either with phase-equivalent unitary transformations or with ad-hoc additive NN interactions.

In the first approach [2], we invoke the power of chiral perturbation theory (ChPT) [3] that provides a promising bridge with the accepted relativistic quantum field theory of the strong interactions, QCD. Beginning with the pionic or the nucleon-pion system [4] one works with systems of increasing nucleon number [5, 6, 7]. One makes use of

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the explicit and spontaneous breaking of chiral symmetry to systematically expand the strong interaction in terms of a characteristic small momentum of a few hundred MeV/c divided by the chiral symmetry breaking scale of about 1 GeV/c. Within the ChPT framework, the NN interactions, the TNI and also πN scattering are related to each other. Results should be trustworthy for observables dominated by momentum scales below this characteristic small momentum and thus, we expect the derived interactions to be valid for low-energy nuclear properties.

We adopt the potentials of ChPT at the orders presently available, N3LO for the NN interaction [8] and N2LO for the TNI [9] . The ChPT expansion divides the interactions into perturbative and non-perturbative elements. The latter are represented by a finite set of constants at each order of perturbation theory that are not presently calculable from QCD but can be fixed by measured properties of nuclei provided the many-body methods are sufficiently accurate. Once the non-perturbative constants are determined, the resulting Hamiltonian predicts, in principle, all other nuclear properties, including those of heavier nuclei with no residual freedom. We refer to this first effort as an application of the *ab initio* NCSM since the NN interaction is completely fixed by properties of the two-body system. Important components of TNI and higher-body interactions are also fixed by the ingredients of the NN terms. Only residual non-perturbatve chiral TNI couplings are fixed, as necessary, by the properties of nuclei beyond $A = 2$. Eventually, independent methods such as lattice QCD should fix all these parameters and complete the *ab initio* NCSM so the need for fitting would be eliminated.

In a second approach [10] the NN interaction is taken as a finite rank separable form in an oscillator representation for each partial wave. The coefficients are determined, to the extent possible, by inverse scattering techniques [11] using the available NN data. Subsequently, one investigates off-shell freedoms with phase-shift equivalent unitary transformations to tune the interaction to fit the properties of light nuclei. By fitting the ^3He and ^{16}O binding energies and the ^6Li low-lying spectra we obtain the interaction "JISP16", which represents "J-matrix Inverse Scattering Potential tuned up to ^{16}O". We achieve soft interactions with this approach that describe all the data conventionally fit by realistic NN interactions and provide good fits to light nuclear properties [10]. We display in Fig. 1 the JISP16 interaction in units of fm for the $^1S_0$ partial wave in momentum space. To obtain units of $MeV\ fm^3$ we multiply by $\frac{\hbar^2}{M_N} = 41.47\ MeV\ fm^2$. Note that this interaction is smooth over the entire range displayed.

We consider this as a phenomenological approach designed to explore regions of NN interactions that are not yet explored by other methods. We hope that the phase-shift equivalent transformation methods that prove successful in this *ab exitu* NCSM will be useful for minimizing higher-body forces in other approaches. This would facilitate efforts to access heavier nuclei within the NCSM. In many instances we find the results of the *ab initio* and *ab exitu* approaches to be similar and we cite the example of ^{10}B in the present work.

In a third approach [12, 13], we supplement the derived realistic effective NN interaction with purely phenomenological terms since the model space is so limited that we expect large corrections from neglected effective interactions such as real and effective TNI's. That is, we surrender the requirement that our effective interactions be entirely derived from the measured NN properties and the theory of many-body potentials. In-

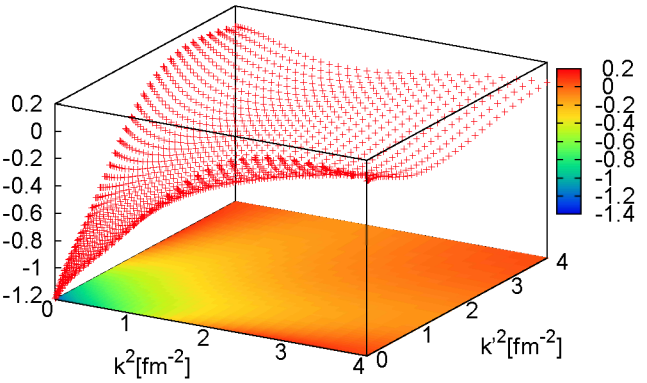

FIGURE 1. JISP16 potential for the $^1S_0$ partial wave in momentum space. The units are fm.

stead, this NCSM approach is patterned after the highly successful phenomenological shell model applied over the years to medium weight nuclei [14, 15]. However, in the NCSM all nucleons are active and we do not input any single-particle energies. That is, we still retain the pairwise interactions between all nucleons and attempt to obtain all properties, including single-particle or mean-field properties, from that pairwise interaction. In this sense, the NCSM is somewhere between the traditional shell model and the Hartree-Fock approach. We present results for ^{47}Ca that illustrate this NCSM approach.

NO CORE SHELL MODEL

The NCSM casts the diagonalization of the infinite dimensional many-body Hamiltonian matrix as a finite matrix in a harmonic oscillator (HO) basis with an equivalent "effective Hamiltonian" derived from the original Hamiltonian [1]. The finite matrix is defined by N_{max}, the maximum number of oscillator quanta shared by all nucleons above the lowest configuration. We solve for the effective Hamiltonian by approximating it as either a 3-body interaction[16] based on our chosen NN+TNI from ChPT (our *ab initio* application) or a 2-body interaction based on JISP16 (our *ab exitu* application). With these "cluster approximations", convergence is guaranteed with increasing N_{max} or with increased cluster size at fixed N_{max} [1].

The NCSM is the only approach currently available to solve the resulting many-body Schrödinger equation for mid-*p*-shell nuclei while preserving all symmetries when the interactions are non-local, a feature of all the interactions employed in this work.

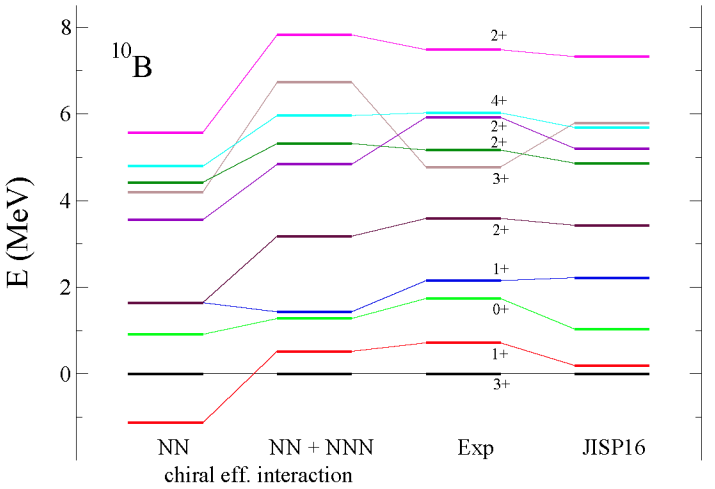

FIGURE 2. Experimental and theoretical excitation spectra of ^{10}B with respect to the lowest 3^+ state at an oscillator energy $\hbar\Omega = 14\,MeV$. The chiral effective interaction results are obtained at $N_{max} = 6$ while the JISP16 results are obtained at $N_{max} = 8$.

Ab initio NCSM with interactions from ChPT

In order to motivate the inclusion of the TNI, we begin by observing that conventional realistic NN interactions do not produce the correct ground state spin of ^{10}B: theory and experiment differ by an inversion of the two lowest levels. This inversion is illustrated in the first column of Fig. 2 for the chiral N3LO potential [8] at an oscillator energy, $\hbar\Omega = 14\ MeV$. Over the past few years, this deficiency, as well as others in mid-p-shell nuclei, such as binding energies, spectral properties and electromagnetic transition rates, have been ascribed to the need for TNI's. In terms of physics, the inadequacy of the realistic NN interactions appears likely to be insufficient spin-orbit splitting in the mean field generated by those interactions, though the mean field itself is not calculated directly. We summarize here the role of the TNI and the role of off-shell modified NN interactions in correcting this inadequacy.

We define the two non-perturbative coupling constants of the TNI, not fixed by 2-body data, as C_D (C_E), the strength of the $N-\pi-NN$ (TNI) contact term. Fig. 3 shows the trajectories of these two parameters as determined from fitting the binding energies of the $A = 3$ & 4 systems as well as the average of the two trajectories. Our approach is similar to the one used in a detailed investigation [17] of ^7Li. The ^4He results use the average of the $A = 3$ fits and the inset shows two crossing points where the ^4He binding is reproduced. Note the expanded scale. The second inset (b) depicts the corresponding rms charge radius of ^4He along with an estimate of the uncertainty in the theory arising from the folding with the proton rms charge radius.

Our results on the radii of the $A = 3$ systems are in good agreement with experiment as well. While the uncertainties in the ^3H and ^3He charge radii obscure the differences between the intersection points, the ^4He charge radius (inset (b) of Fig. 3) indicates a

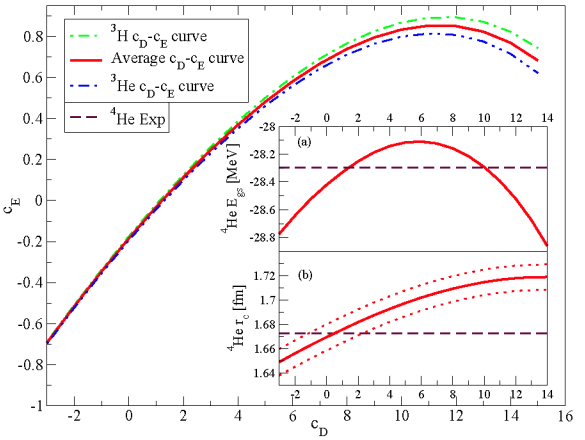

FIGURE 3. Relations between C_D and C_E for which the binding energy of ^{3}H (8.482 MeV) and ^{3}He (7.718 MeV) are reproduced. (a) ^{4}He binding energy along the averaged curve. The experimental ^{4}He binding energy (28.296 MeV) defines two points of intersection using the averaged $A = 3\,C_D - C_E$ curve. (b) ^{4}He charge radius. Dotted lines represent the spread in r_c due to uncertainties in the proton charge radius.

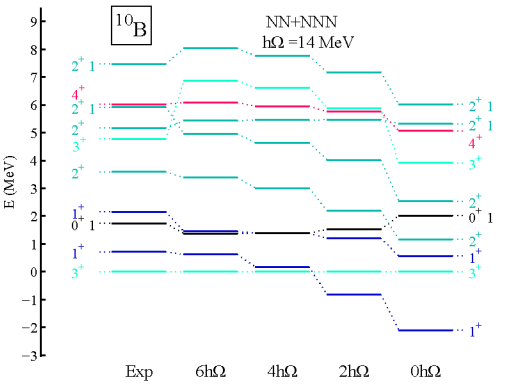

FIGURE 4. Experimental and theoretical excitation spectra of ^{10}B with respect to the lowest 3^+ state. The NCSM results are obtained with the chiral NN + TNI interaction [8, 9] at an oscillator energy, $\hbar\Omega = 14\ MeV$ as a function of N_{max} indicated at the bottom of each spectrum. Note the reasonable convergence as one proceeds up to $N_{max} = 6$

preference for $C_D \sim 0$ with a broad span of reasonable results around it. This led us to investigate observables in the mass 10-13 range where we find good results for $C_D = -1$, $C_E = -0.33$ [2].

An example of the improvement obtained with the TNI of ChPT for these values of C_D and C_E is shown in Fig. 2. The correct level ordering is now obtained for the lowest 5

states. In addition, the binding energy shifts towards agreement with experiment as seen below in Table 1. Refinements in our numerical methods will soon allow us to obtain the spectrum at $N_{max} = 8$ to extend the convergence trends for Fig. 4.

Ab exitu: NCSM with interaction from inverse scattering

Turning to results with the *ab exitu* NCSM we present in Fig. 2 a sample comparison of results with the *ab initio* NCSM for ^{10}B. We note that both approaches yield the correct level ordering through the first five states. Similar favorable comparisons are found in other light nuclei. It will be very helpful to have results for both approaches in larger basis spaces in order to asses more completely the distinctions between these approaches.

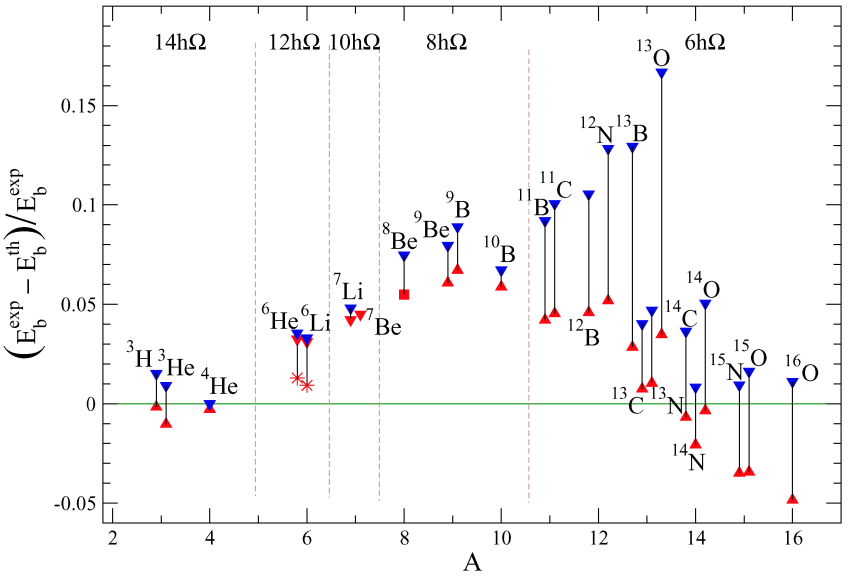

FIGURE 5. Fractional difference between theory and experiment for the binding energies of stable p-shell nuclei. The results are quoted with the specified N_{max} values and with both the bare and effective JISP16 interactions. The effective interactions are evaluated at the 2-body cluster level. The oscillator energy, $\hbar\Omega$ is taken, in each case, to be the value at which an extremum in the binding energy occurs.

For a more comprehensive view of the results with the *ab exitu* calculations, we present in Fig. 5 the binding energies of stable p-shell nuclei relative to experiment using the JISP16 interaction. Both bare and effective interaction results are presented as well as some initial extrapolations to the infinite basis limit [18]. The bare interaction results are strict upper bounds to the exact ground state energy so the bare curves will drop as the basis space is increased (direction of increased binding in the theory). The effective interaction results do not follow a variational principle. The results show a tendency to underbind nuclei in mid-p-shell and to overbind at the upper end by a few percent. Results in larger basis spaces will help clarify these trends.

Full Configuration Interaction calculations

As an alternative to deriving an effective finite many-body Hamiltonian matrix from the original Hamiltonian using the Lee-Suzuki method [1], one can solve the finite matrix defined by N_{max} for the original Hamiltonian. This has the benefit that the variational principle applies, and thus the binding energy obtained for a finite value of N_{max} is a strict upper bound for the converged result. In addition, the approach to convergence is monotonic, facilitating extrapolation techniques to infinite model-spaces. This constitutes a full Configuration Interaction (FCI) method.

In Fig. 6 we present initial results for the ground state energy of ^{12}C in an $N_{max} = 8$ basis space using the original (bare) JISP16 interaction and compare with the results obtained in smaller basis spaces. While the convergence trend is encouraging, see Fig. 7, we note that JISP16 produces a small amount of overbinding as indicated by our preliminary extropolated ground state energy and its uncertainty [18].

The convergence rate of a FCI calculation depends on the interaction: For soft interactions such as JISP16, this works quite well [18]; for other interactions convergence can be improved by a suitable renormalization of the Hamiltonian [19]. As further indication of the value of FCI, we note that other observables, such as the point proton rms radius, may be evaluated directly. Results for ^4He show excellent convergence to a result very close to experiment [18].

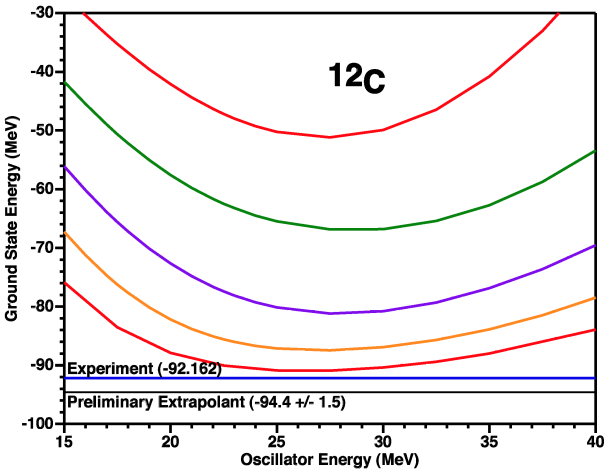

FIGURE 6. Ground state energy for ^{12}C as a function of the oscillator energy, $\hbar\Omega$, for $N_{max} = 0 - 8$ for the bare JISP16 interaction. The $N_{max} = 8$ curve is closest to experiment and each curve above it corresponds to decreases in N_{max} by two units.

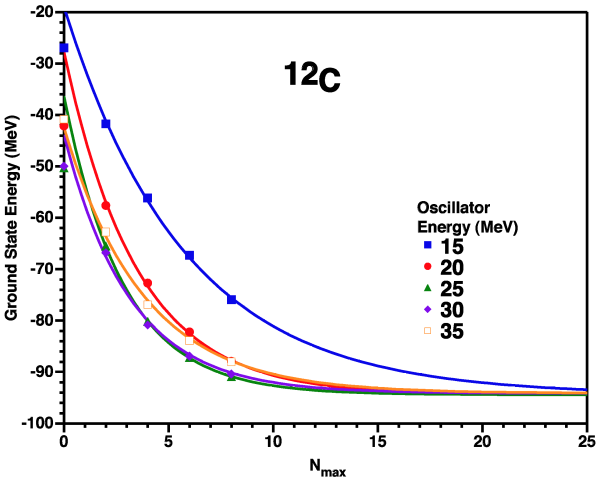

FIGURE 7. Calculated ground state energy of ^{12}C for $N_{max} = 0 - 8$ at selected values of $\hbar\Omega$. The data for $N_{max} = 2 - 8$ are fit to an exponential for each $\hbar\Omega$ plus a common constant, the asymptote. The preliminary result for the asymptote is $-94.4 \pm 1.5\ MeV$ compared with the experimental ground state energy $-92.16\ MeV$. The uncertainty is assigned using the range of the asymptotes from independent fits to the four points at each value of $\hbar\Omega$ shown here.

NCSM with interaction from theory and phenomenology

In the third approach, we work towards heavier nuclei and must restrict ourselves to basis spaces that are far from convergence as seen from the trends in light nuclei. Hence, we adopt a more phenomenological approach to the input Hamiltonian. Motivated by the success of the conventional shell model and by our successes in light nuclei, we fashion a hybrid approach that retains features of both - in particular the features that all nucleons are active and the feature that the NN interaction is adjusted to fit the properties of the heavier nuclei [12, 13].

In brief, the results are the following [12]: i) one finds that the charge dependence of the bulk binding energy of eight A=48 nuclei is reasonably described with an effective Hamiltonian derived from CD-Bonn interaction[22], while there is an overall underbinding by about 0.4 MeV/nucleon; ii) the resulting spectra are too compressed compared with experiment; iii) when isospin-dependent central NN terms plus a tensor NN interaction are added to the Hamiltonian, one achieves accurate total binding energies for eight A=48 nuclei and reasonable low-lying spectra for the three nuclei involved in double-beta decay. Only five input data were used to determine the phenomenological terms - the total binding of ^{48}Ca, ^{48}Sc, and ^{48}Ti along with the lowest positive and negative parity excitations of ^{48}Ca.

We have extended this approach to the odd-A isotopes ^{47}Ca, ^{49}Ca, ^{47}Sc and ^{47}K [13], which differ by one nucleon from ^{48}Ca. One of our goals is to test whether the same

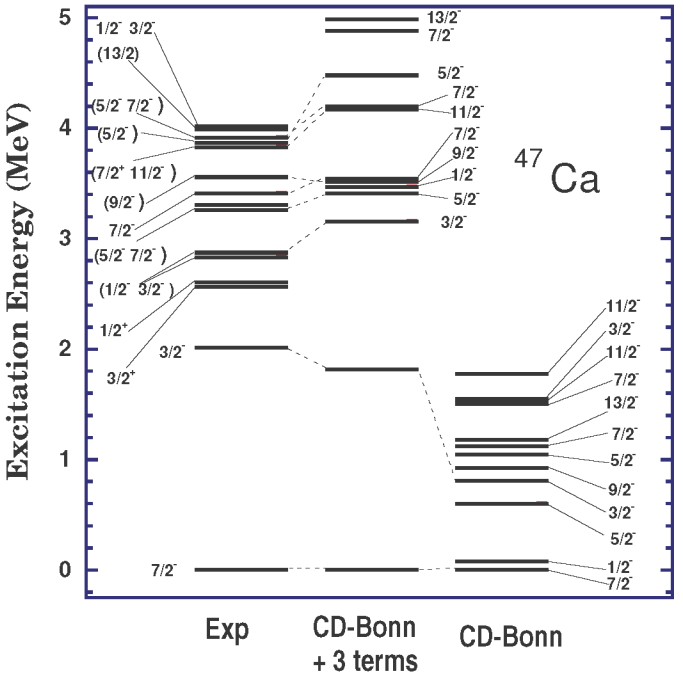

FIGURE 8. Experimental and theoretical excitation energy levels for ^{47}Ca. Both CD-Bonn and CD-Bonn+3terms results are presented.

modified effective Hamiltonian used for A=48 isotopes, is able to describe these odd-A nuclei. A particular feature of the spectroscopy of these odd nuclei is that the spin-orbit splitting gives rise to a sizable energy gap in the fp-shell between the $f_{7/2}$ and other orbitals ($p_{1/2}$, $p_{3/2}$, $f_{5/2}$) and we wanted to see if this feature can be reproduced in a NCSM where we have no input single-particle energies. The results both with and without the phenomenological terms are presented in Fig. 8.

In spite of the differences in frameworks with and without a core, we also wanted to compare our initial and modified Hamiltonian with a recent fp-shell interaction, the GXPF1, developed by Honma, Otsuka, Brown and Mizusaki [23]. We feel it is valuable to compare various fp-shell interactions in order to understand better their shortcomings and their regimes of applicability. From that comparison, notable differences are evident. For example, our diagonal two-body T=0 matrix elements are more attractive and, while our initial and modified NN Hamiltonian fp-shell matrix elements are strongly correlated, there is much less correlation with the GXPF1 matrix elements. It is worth mentioning that our interaction and Honma et al. GXPF1 interactions were also tested recently within the framework of spectral distribution theory in Ref. [24] and sizable differences were demonstrated.

TABLE 1. Properties of ^{10}B from experiment and theory. E2 transitions are in e^2 fm^4 and M1 transitions are in μ_N^2. The rms deviations of excited state energies are quoted for the lowest 9 states whose spin-parity assignments are well established and that are known to be dominated by $0\hbar\Omega$ configurations. Results are obtained in the basis spaces $N_{\max} = 6(8)$ with $\hbar\Omega = 14$ MeV for the ChPT (JISP16) interaction. In the $N3LO + TNI$ column we show selected sensitivity to changing C_D by ± 1. "N/A" indicates a result yet to be calculated. The experimental values are from Ref. [20, 21].

Property	**Exp**	***N3LO +TNI***	***N3LO***	***JISP16***
$\lvert E(3^+,0)\rvert$ [MeV]	64.751	64.78	56.11	59.751
r_p [fm]	2.30(12)	2.197	2.256	2.210
$Q(3_1^+,0)$ [e fm^2]	+8.472(56)	+6.327	+6.803	6.716
$\mu(3_1^+0)$ [μ_N]	+1.801	+1.837	+1.853	N/A
$E_x(3_1^+0)$ [MeV]	0.0	0.0	0.0	0.0
$E_x(1_1^+0)$ [MeV]	0.718	0.523	-1.128	0.193
$E_x(0_1^+1)$ [MeV]	1.740	1.279	0.913	1.034
$E_x(1_2^+0)$ [MeV]	2.154	1.432	1.643	2.221
$E_x(2_1^+0)$ [MeV]	3.587	3.178	1.643	3.430
$E_x(3_2^+0)$ [MeV]	4.774	6.729	4.193	5.792
$E_x(2_1^+1)$ [MeV]	5.164	5.315	4.419	4.861
$E_x(2_2^+0)$ [MeV]	5.92	4.835	3.555	5.201
$E_x(4_1^+0)$ [MeV]	6.025	5.960	4.790	5.685
$E_x(2_2^+1)$ [MeV]	7.478	7.823	5.565	7.320
$rms(Exp-Th)$ [MeV]	-	0.823	1.482	0.536
B(E2;$1_1^+0 \to 3_1^+0$)	4.13(6)	3.05(62)	4.380	3.736
B(E2;$1_2^+0 \to 3_1^+0$)	1.71(0.26)	0.50(50)	0.082	0.578
B(M1;$2_1^+0 \to 3_1^+0$)	0.0015(3)	0.0000	N/A	0.0012
B(M1;$2_1^+1 \to 3_1^+0$)	0.041(4)	0.216	N/A	0.125
B(M1;$2_2^+0 \to 3_1^+0$)	0.050(12)	0.053	N/A	0.056
B(M1;$4_1^+0 \to 3_1^+0$)	0.043(7)	0.002	N/A	0.003
B(M1;$2_2^+1 \to 3_1^+0$)	-	4.020	N/A	4.148
B(GT;$3_1^+0 \to 2_1^+1$)	0.083(3)	0.07(1)	0.102	0.040
B(GT;$3_1^+0 \to 2_2^+1$)	0.95(13)	1.22(2)	1.487	1.241

CONCLUDING REMARKS

Table 1 contains selected experimental and theoretical results for ^{10}B. The binding energy and rms deviation between the experimental and theoretical excitation energies improve substantially with the inclusion of TNI. The JISP16 results lie intermediate to the N3LO and N3LO+TNI interaction results. Other observables are in reasonable accord with experiment considering that (1) we use bare electromagnetic operators, and (2) moments and transition rates are expected to be more sensitive to enlarging the basis spaces as we plan to do. The JISP16 results employ partial waves, $J \leq 4$. If we retain only $J \leq 3$ partial waves in JISP16, the excitation energies change by less than 10 keV and the binding energy decreases by 35 keV.

These results required substantial computer resources. The $N_{max} = 6$ spectrum shown in Fig. 4 and a set of additional experimental observables, takes an hour on 3500

processors on the LLNL-Thunder machine. Our largest run that is reported here, the ^{12}C with JISP16 in the $N_{max} = 8$ basis ($dimension = 6 \times 10^8$) took 2.3 hours on 15,400 processors (33,350 cpu hours) at the ORNL Jaguar facility for a single $\hbar\Omega$ value. All runs produce the lowest 15 converged eigenvectors and a suite of observables (rms radii, electromagnetic moments and transitition rates, electroweak transition rates, etc.). Development efforts underway promise to reduce the computational time by about a factor of two and to facilitate enhanced convergence as well as reaching heavier systems.

We demonstrated here that TNI's make substantial contributions to improving the spectra and other observables. In addition, phase-equivalent transformations of an interaction obtained from inverse scattering, JISP16, produces appealing fits to light nuclear properties. However, there is considerable room for further improvement in both approaches. Our leading suggestions include: (1) extend the TNI's to the order consistent with the NN interaction, N3LO; (2) extend the basis spaces to higher N_{max} values to further improve convergence; (3) examine sensitivity of TNI's to the choice of regulator; and (4) include four-nucleon interactions at a consistent order of ChPT. In addition, further exploration of the phase-shift equivalent transformations appears warranted. Finally, improving the phenomenological fits to medium mass nuclei appears within reach.

Our overall conclusion is that these results support a full program of deriving the NN interaction and its mulit-nucleon partners in the consistent approach provided by chiral effective field theory. It is straightforward, but challenging, to extend this research thrust in the directions indicated. However, the favorable results to date and the need for addressing fundamental symmetries of strongly interacting systems with enhanced predictive power firmly motivate this path. Recent developments of techniques to achieve physically-motivated larger basis spaces [25] hold great promise for attaining many of the goals we seek.

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