Light nuclei and NN interaction obtained in the J-matrix inverse scattering approach

A M Shirokov†, J P Vary‡, A I Mazur§, S A Zaytsev§ and T A Weber‡
† *Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow, 119992, Russia*
‡ *Department of Physics and Astronomy, Iowa State University, Ames, Ia 50011-3160, USA*
§ *Physics Department, Khabarovsk State Technical University, Tikhookeanskaya 136, Khabarovsk 680035, Russia*

Abstract

A nucleon-nucleon interaction is constructed by means of the J-matrix version of inverse scattering theory as a set of small-rank matrices in the oscillator basis. Phase-equivalent transformations are used to fit the interaction to the properties of light nuclei. The resulting interaction, JISP6, accurately reproduces the NN scattering data, deuteron properties and spectroscopy of $A \leq 6$ nuclei within the no-core shell model.

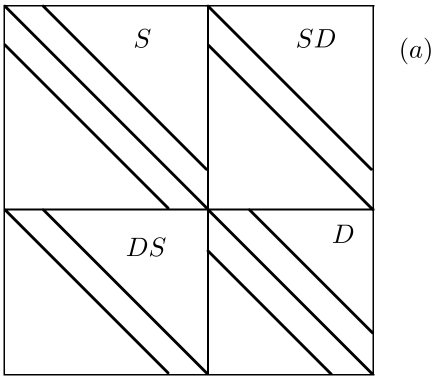
Nucleon-nucleon (NN) potentials that describe available two-body data have a long and multi-faceted history. High precision fits have improved with time even as more precise experimental data have become available. Three-nucleon (NNN) potentials have a shorter history but are intensively investigated at the present time. Disparate foundations for these potentials, both NN and NNN, have emerged. There are meson-exchange potentials sometimes supplemented with phenomenological terms to achieve high accuracy in fitting NN data (Bonn [1], Nijmegen [2], Argonne [3], Idaho [4], INOY [5]) and NNN data (Urbana [6, 7], Illinois [8], Tucson–Melbourne [9, 10]). On the other hand, one sees the emergence of potentials with ties to QCD which are either meson-free [11], or intertwined with meson-exchange theory [12, 4]. All these potentials are being used, with unprecedented success, to explain a vast amount of data on light nuclei in Quantum Monte Carlo approaches [7] and *ab initio* no-core shell model (NCSM) [13, 14, 15].

Chief among the outstanding challenges is the computational intensity of using these $NN+NNN$ potentials within the presently available many-body methods. For this reason, most *ab initio* investigations have been limited to $A \leq 12$. The situation would be dramatically simpler if either the NN potential alone would be sufficient or the potentials would couple less strongly between the low momentum and the high momentum degrees of freedom. If both simplifications are obtained, the future for applications is far more promising.

Recently [16, 17] we derived a new class of NN potentials that have no apparent connection with the two well-established lines of endeavor. We developed J-matrix inverse scattering potentials (JISP) that describe NN data to high accuracy and, with the off-shell freedom that remains, we obtain excellent fits to the bound and resonance states of light nuclei up to $A = 6$. Our NN off-shell freedom is sufficient to describe these limited data without the need for NNN potentials. As an important side benefit, we find that these potentials lead to rapid convergence in the *ab initio* NCSM calculations. We hope that these potentials will open a fruitful path for evaluating heavier systems and spur the development of extensions to scattering problems.

Our NN potentials have the same symmetries as the conventional NN potentials mentioned above (without charge symmetry breaking at present), but are not constrained by meson exchange theory, by QCD or by locality. This does not mean our NN potentials are inconsistent with those constraints, however. Indeed, we claim consistency with the meson exchange theory and QCD in so far as these constraints are embodied in the experimental data we fit. For example, conventional wisdom says that the NN phase shifts and deuteron properties cannot be fit to high precision without a long-range one-pion exchange potential. The NN scattering data have even been used [18] to extract rather precise values of the pion mass, indicating the NN data tightly constrains the long-range part of the interaction.

By means of the J-matrix inverse scattering approach [19, 20, 21] we construct NN potentials as matrices in an oscillator basis using the Nijmegen np phase shifts [22]. First, using the technique described in detail in [16], we obtain inverse scattering tridiagonal potentials (ISTP). These potentials have tridiagonal matrices in uncoupled partial waves; in coupled partial waves the matrices of the ISTP interaction are quasi-tridiagonal as is illustrated by Fig. 1 (a). The dimension of the potential matrix is specified by the maximum value of $N = 2n + l$ and is referred to as an $N\hbar\omega$ potential. We develop $9\hbar\omega$-ISTP in odd



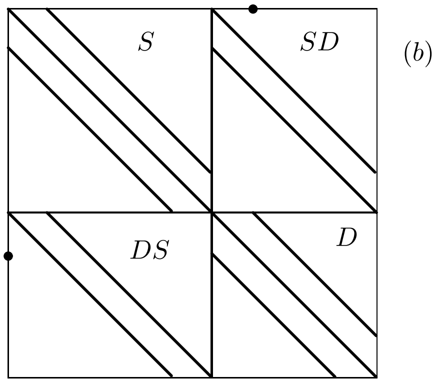


Figure 1: Structure of the initial quasi-tridiagonal ISTP matrix (a) in the coupled SD waves and the JISP matrix (b) obtained from the ISTP matrix by means of PET. The location of non-zero matrix elements is schematically illustrated by thick lines and filled circles.

waves and $8\hbar\omega$-ISTP in the even partial waves. A high quality description of the two-body data with these low values of N is obtained with $\hbar\omega = 40$ MeV. As an example, we present in Fig. 2 our description of the δ_p, δ_f phase shifts and the mixing parameter ε_2 in the coupled pf waves in comparison with the Nijmegen-II potential predictions. It seen from the figure that the $9\hbar\omega$-ISTP better reproduces the data than the $7\hbar\omega$-ISTP.

Next we perform various phase equivalent transformations (PETs) of the obtained ISTP. PETs do not affect the phase shifts and mixing parameters, however with the help of PETs we improve predictions for other observables. In particular, applying PET in the coupled sd waves, we fit the interaction to the deuteron rms radius r_d and quadrupole moment Q. The description of the deuteron properties (the ground state energy E_d, the d state probability P_D, r_d, Q, the s wave asymptotic normalization constant $\mathscr{A}_S$ and the ratio of the asymptotic normalization constants $\eta = \mathscr{A}_D/\mathscr{A}_S$) is compared with the predictions of other realistic potentials in Table 1. It is interesting that the NN interaction in sd coupled waves fitted in our approach to the deuteron quadrupole moment, provides very accurate predictions for the ^{3}H and ^{4}He binding energies, much better than with other realistic NN potentials and comparable with the ones obtained with modern $NN + NNN$ potential models. The ^{3}H and ^{4}He binding energies are very slightly affected by the PETs in other partial waves. At the same time, the binding energies and spectra of the p shell nuclei are very sensitive to the PETs in all p waves and in some of d waves. Therefore the p shell spectroscopy provides us with a new information for the tuning of the NN interaction.

The potentials obtained by means of PETs from the initial ISTP interaction are refered to as JISP. Fitting PET parameters to the spectrum of the ^{6}Li nucleus, we obtain the JISP6 interaction, i. e. the JISP interaction fitted to the spectra of $A \leq 6$ nuclei.

PETs are generated by unitary transformations of the Hamiltonian matrix with the respective ISTP; the matrices of these unitary transformations in the oscillator basis are of the type

$$[U] = [U_0] \oplus [I] = \left[\begin{array}{c|c} [U_0] & 0 \\ \hline 0 & [I] \end{array}\right], \tag{1}$$

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

Potential	E_d (MeV)	P_D (%)	r_d (fm)	Q (fm^2)	$\mathscr{A}_S$ (fm$^{-1/2}$)	η
JISP6	-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)

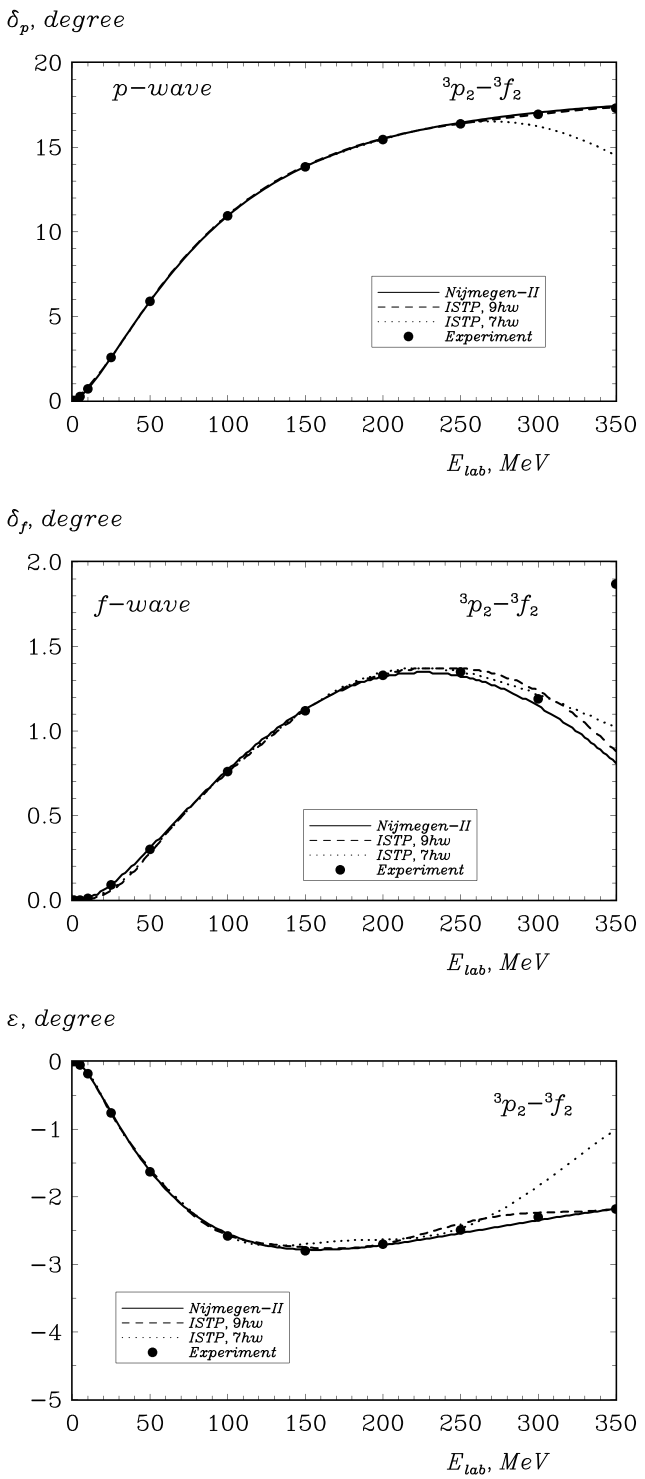


Figure 2: np scattering phase shifts δ_p, δ_f and mixing parameter ε_2 in the coupled pf waves

Table 2: The binding energies of light nuclei obtained with JISP6 in NCSM with $\hbar\omega = 15$ MeV in comparison with the results obtained with modern $NN+NNN$ interaction models in various approaches.

Potential, approach	^{3}H	^{3}He	^{4}He	^{6}He	^{6}Li
JISP6, NCSM	8.461(5)	7.751(3)	28.611(41)	29.24(17)	31.48(27)
CD-Bonn+TM, Faddeev [23]	8.480	7.734	29.15		
AV18+TM, Faddeev [23]	8.476	7.756	28.84		
AV18+TM, Faddeev [23]	8.444	7.728	28.36		
Nijmegen-I+TM, Faddeev [23]	8.392	7.720	28.60		
Nijmegen-II+TM, Faddeev [23]	8.386	7.720	28.54		
AV18+UIX, Faddeev [23]	8.478	7.760	28.50		
AV18+UIX, GFMC [7]	8.47(1)		28.30(2)	27.64(14)	31.25(11)
AV8′+TM′, NCSM [15]				28.189	31.036
Nature	8.48	7.72	28.30	29.269	31.995

where $[I]$ is the infinite unit matrix (see [16] for more details). We take the simplest form of the only non-trivial submatrix $[U_0]$ of the matrix (1): a 2×2 rotation matrix with a single continuous parameter ϑ coupling the the lowest basis oscillator functions $|0LSJ\rangle$ and $|1LSJ\rangle$ with the same values of L, S and J in all cases except the case of the coupled sd waves where the matrix $[U_0]$ mixes the lowest oscillator functions $|0s\rangle$ and $|0d\rangle$,

$$[U_0] = \begin{bmatrix} U_{00}^{ss} & U_{00}^{sd} \\ U_{00}^{ds} & U_{00}^{dd} \end{bmatrix} = \begin{bmatrix} \cos\vartheta & +\sin\vartheta \\ -\sin\vartheta & \cos\vartheta \end{bmatrix}. \tag{2}$$

As a result, the potential matrix acquires two additional non-zero matrix elements $V_{01}^{sd} = V_{10}^{ds}$ which are schematically illustrated by filled circles in Fig. 1 (b). The JISP6 interaction is obtained with the PET parameters $\vartheta = -11.3°$, $+8°$, $-6°$, $+25°$ and $-16°$ in the coupled sd, $^3p_2$, $^3p_1$, $^3d_2$ and $^1p_1$ waves respectively. The matrix elements of the JISP6 interaction can be found in Ref. [17].

The calculations of light nuclei are performed in the NCSM with JISP6 plus the Coulomb interaction between protons. To improve the convergence, we perform the Lee–Suzuki transformation to obtain a two-body effective interaction as is discussed in [14]. The effective interaction is obtained in a new oscillator basis with $\hbar\omega = 15$ MeV within an $N_{max}\hbar\omega$ model space where N_{max} signifies the many-body oscillator basis cutoff. The results of our NCSM calculations for binding energies of ^{3}H, ^{3}He (in the $14\hbar\omega$ model space), ^{4}He (in the $12\hbar\omega$ model space), ^{6}He and ^{6}Li (in the $10\hbar\omega$ model space) nuclei are compared in Table 2 with the calculations in various approaches [Faddeev, Green's-function Monte Carlo (GFMC), NCSM] with realistic NN [CD-Bonn, Nijmegen-I, Nijmegen-II, Argonne (AV18 and AV8′)] and NNN [Urbana (UIX), Tucson–Melbourne (TM and TM′)] potentials. To give an estimate of the convergence of our calculations, we present the difference between the given result and the result obtained in the next smaller model space in parenthesis after our JISP6 results. It is seen that the convergence of our calculations is adequate.

The convergence patterns are also illustrated by Fig. 3 where we present the $\hbar\omega$ dependence of the ^{6}Li ground state energy in comparison with the results of reference [24] obtained in NCSM with CD-Bonn interaction. The $\hbar\omega$ dependence with the JISP6 interaction is weaker over a wide interval of $\hbar\omega$ values. This is a signal that the convergence is improved relative to CD-Bonn. The variational principle cannot be applied to the NCSM calculations with effective interactions so the convergence may be either from above or below. However, we may surmise that the residual contributions of neglected three-body effective interactions is more significant in the CD-Bonn case.

The $\hbar\omega$ dependence of lighter nuclei is even weaker. That is why we present the results for all nuclei obtained with the same $\hbar\omega$ value. In this case the difference between ground state energies provide a consistent predictions for reaction Q values.

Returning to the results presented in Tables 1–2, we see that the JISP6 interaction provides a realistic description of the ground states of light nuclei competitive with the quality of descriptions previously achieved with both NN and NNN forces.

This conclusion is supported by the spectra and ground state properties of $A = 6$ nuclei summarized in

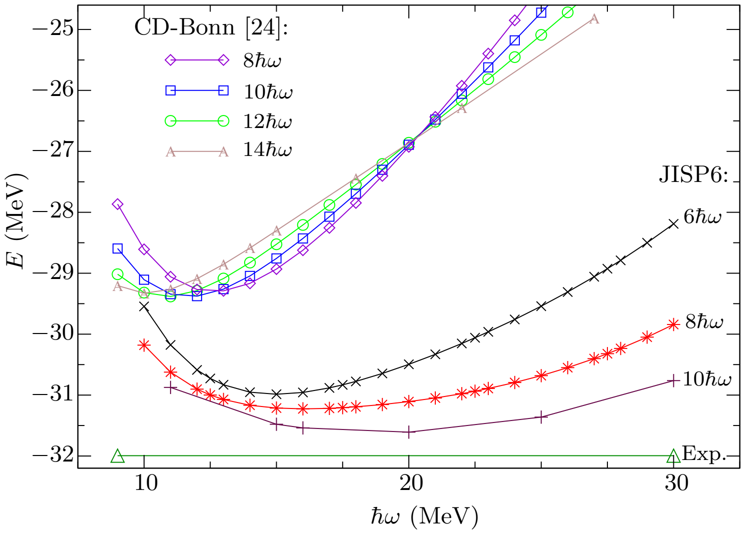


Figure 3: $\hbar\omega$ dependence of the ^{6}Li ground state energy obtained with JISP6 interaction in comparison with the one obtained in [24] in NCSM with CD-Bonn potential.

Table 3. We again present in parenthesis the difference between the given value and the result obtained in the next smaller model space. Note that the ^{6}Li spectrum was found [15] to be sensitive to the presence of the NNN force and a high-quality description of the ^{6}Li spectrum seemed impossible without NNN forces. It is seen that the ^{6}Li spectrum is well-reproduced in our calculations and competitive with realistic $NN + NNN$ models. The most important difference with the experiment is the excitation energy of the $(1_2^+, 0)$ state. However $E_x(1_2^+, 0)$ goes down rapidly when the model space is increased and better results are anticipated in a larger model space.

The point-proton rms radius r_p and the quadrupole moment Q have a more prominent $\hbar\omega$ dependence than the binding energy. $\hbar\omega = 15$ MeV is not the optimal value for these observables in $A = 6$ nuclei and hence their convergence is not very good. The exponential extrapolation of the ^{6}Li point-proton rms radius using the results obtained with different $\hbar\omega$ values results in the value of $r_p \approx 2.14$ fm. The ^{6}Li quadrupole moment Q 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, various cluster model calculations cannot reproduce even the negative sign of Q. Our results for Q are seen to be competitive with the ones obtained with $NN + NNN$ potentials.

We return to the underlying rationale for our approach and ask why it is conceivable that an NN interaction alone may be competitive with the $NN + NNN$ potentials mentioned at the outset. That this is feasible may be appreciated from the theorem of Polyzou and Glöckle [25]. They have shown that changing the off-shell properties of two-body potentials is equivalent to adding many-body interactions. This theorem coupled with our limited results suggests that our inverse scattering NN potential plus off-shell modifications is roughly equivalent, for the observables so far investigated, to the successful $NN + NNN$ potential models.

Clearly, it is very interesting to extend this approach to heavier nuclei. Our preliminary calculations show that the JISP6 interaction provides reasonable results for the nuclei with $A < 10$ but overbinds the p shell nuclei with $A \geq 10$. However this drawback can be eliminated by a slight modification of the PET parameters ϑ. This work is in progress and we hope to publish soon the JISP16 interaction fitted to nuclei with $A \leq 16$.

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Table 3: Excitation energies E_x (in MeV) and ground state point-proton rms radii r_p (in fm) and quadrupole moments Q (in $e \cdot \mathrm{fm}^2$) of $A = 6$ nuclei.

^{6}Li

Potential Approach	Nature	JISP6 NCSM, $10\hbar\omega$	AV8′+TM′ NCSM, $6\hbar\omega$ [15]	AV18+UIX GFMC [7]
$E_x(1_1^+,0)$	0.0	0.0	0.0	0.0
r_p	2.32(3)	2.083(25)	2.054	2.46(2)
Q	0.082(2)	0.194(55)	0.025	0.33(18)
$E_x(3^+,0)$	2.186	2.102(4)	2.471	2.72(36)
$E_x(0^+,1)$	3.563	3.348(24)	3.886	3.94(23)
$E_x(2^+,0)$	4.312	4.642(2)	5.010	4.43(39)
$E_x(2^+,1)$	5.366	5.820(4)	6.482	
$E_x(1_2^+,0)$	5.65	6.86(36)	7.621	

^{6}He

Potential Approach	Nature	JISP6 NCSM, $10\hbar\omega$	AV8′+TM′ NCSM, $6\hbar\omega$ [15]	AV18+UIX GFMC [7]
$E_x(0^+,1)$	0.0	0.0	0.0	0.0
r_p	1.912(18)	1.694(3)	1.707	1.95(1)
$E_x(2^+,1)$	1.8	2.505(86)	2.598	1.80(18)

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