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Theory

Spectroscopy of Light Nuclei with Realistic *NN* Interaction JISP

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Abstract—Recent results of our systematic ab initio studies of the spectroscopy of s- and p-shell nuclei in fully microscopic large-scale (up to a few hundred million basis functions) no-core shell-model calculations are presented. A new high-quality realistic nonlocal NN interaction JISP is used. This interaction is obtained in the J-matrix inverse-scattering approach (JISP stands for the J-matrix inverse-scattering potential) and is of the form of a small-rank matrix in the oscillator basis in each of the NN partial waves, providing a very fast convergence in shell-model studies. The current purely two-body JISP model of the nucleon–nucleon interaction JISP16 provides not only an excellent description of two-nucleon data (deuteron properties and np scattering) with $\chi^2/\text{datum} = 1.05$ but also a better description of a wide range of observables (binding energies, spectra, rms radii, quadrupole moments, electromagnetic-transition probabilities, etc.) in all s- and p-shell nuclei than the best modern interaction models combining realistic nucleon–nucleon and three-nucleon interactions.

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A number of high-precision fully microscopic approaches in the theory of nuclear structure that do not involve any model-dependent assumptions (for example, the concept of an inert core) have been developed in recent years; they are commonly known as ab initio approaches. Of course, the possibility of performing ab initio calculations is predicated on the development of supercomputers and is currently restricted to comparatively light nuclei. Ab initio methods include approaches based on numerically solving Faddeev and Faddeev–Yakubovsky equations in the theory of few-body systems and, in the case of heavier nuclei, some modern versions of the Monte Carlo method (variational Monte Carlo and Green's function Monte Carlo methods), the method of hyperspherical functions, the coupled-cluster approach, and some modern versions of the shell model. We believe the no-core shell model (NCSM) [1] to be currently the most promising ab initio method that makes it possible to perform high-precision studies of $A \geq 6$ nuclei.

The nucleon–nucleon interaction exhausts input information for ab initio investigations in nuclear theory. At the present time, there are a number of high-precision, so-called realistic, NN interactions relying on meson-exchange theory and providing a perfect description of deuteron properties and data on NN scattering. It is well known that such interactions not supplemented with three-nucleon forces fail to describe the binding energies of the light nuclei ^{3}H, ^{3}He, and ^{4}He (they are calculable precisely by various methods), as well as some features of heavier nuclei—for example, the ground-state spin of the ^{10}B nucleus. Usually, three-nucleon forces whose parameters are fitted to the binding energies of one or a few extremely light nuclei (or, sometimes, to a wider range of nuclear properties) are introduced to improve the situation. However, the inclusion of three-nucleon forces substantially complicates microscopic calculations, imposing much more stringent requirements on the computational resources and increasing the time of the calculations. All this constrains substantially the range of nuclei amenable to investigations and the possibilities for extending the model space, thereby reducing the accuracy of the calculations.

There arises the question of whether it is possible to describe the properties of at least light nuclei without three-nucleon forces and to preserve simultaneously the precision level ensured by modern realistic potentials in describing deuteron properties and NN scattering data. A hope for a positive answer was inspired by the results obtained in [2], where it was shown that, upon subjecting a two-body NN interaction to phase-equivalent transformations, the spectrum and the binding energy of the original three-body system governed by a purely two-body NN

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interaction are equivalent to the spectrum and the binding energy of a three-body system governed by the resulting two-body NN interaction subjected to a phase-equivalent transformation and supplemented with a three-nucleon interaction. Unfortunately, there is no inverse theorem stating that a system governed by a two-body interaction combined with any three-body interaction can always be equivalently described by using only some two-body interaction obtained from the original one by means of a phase-equivalent transformation. Nevertheless, the theorem proven in [2] gives grounds to assume that one can at least reduce the role of three-nucleon forces in the system by applying phase-equivalent transformations to the NN interaction.

In this study, we use a realistic NN interaction obtained within the J-matrix inverse-scattering approach proposed in [3]. This interaction is constructed in the form of small-rank matrices in the harmonic-oscillator basis. Not only is this form convenient for various applications of the shell model, but it also ensures a rapid convergence of shell-model calculations. This interaction provides a description of two-body NN data that has an accuracy comparable with the accuracy of the best modern NN potentials: for our potential, χ^2/datum, a standard measure of the accuracy of NN potentials, is 1.03 for the 1992 np database (2514 data) and 1.05 for the 1999 np database (3058 data) [4]. We apply the phase-equivalent transformations proposed in [3, 5] to this interaction and perform NCSM calculations for light nuclei, trying to fit the parameters of the phase-equivalent transformations to the spectra and binding energies of the nuclei being considered without resort to three-nucleon forces. It turned out that the preceding version of this interaction, JISP6 [5], fitted to the properties of $A \leq 6$ nuclei, led to a strong overbinding of $A \geq 10$ nuclei. In view of this, we performed a new search for the parameters of phase-equivalent transformations and arrived at a new interaction version, JISP16 [4], which made it possible to describe the properties of $A \leq 16$ nuclei. In order to save computer time, the interaction was fitted in comparatively small NCSM model spaces (for example, $10\hbar\omega$ and $4\hbar\omega$ for the ^{6}Li and ^{16}O nuclei, respectively). The results presented below were obtained with the JISP16 NN interaction by using larger model spaces without any additional fit—that is, within an essentially ab initio approach. The matrix elements of the JISP16 interactions can be found in [4].

Let us first discuss the results of our calculations for the binding energies of s- and p-shell nuclei in Table 1. As a rule (see, for example, [1]), NCSM calculations are performed with effective interactions constructed by applying the Lee–Suzuki transformation to the original NN interaction (in our case, this is JISP16 supplemented, of course, with the Coulomb interaction of protons), the convergence being substantially improved in this way. Moreover, the specific form of the JISP16 interaction ensures a rather high rate of convergence even in the case of the "bare" (not transformed) interaction; in many cases, this makes it possible to specify confidence intervals for our NCSM predictions.

According to the variational principle, the results of NCSM calculations for the binding energies of nuclei with the bare JISP16 interaction always converge from below. However, the variational principle is inapplicable to calculations with the effective interaction. For the majority of s- and p-shell nuclei, the results of NCSM calculations for the binding energies with the effective interaction based on JISP16 converge from above. In such cases, the results obtained with the bare and the effective interaction provide the boundaries of the confidence interval for our predictions of the binding energies of nuclei. We note that, for $6 \leq A \leq 8$ nuclei, the results of the calculations with the effective interaction converge from below; for this reason, the results obtained with the bare interaction, in which case the convergence is poorer, are not presented in Table 1.

To illustrate the convergence rate, the differences of the displayed results and the respective results obtained in the nearest NCSM model space of smaller size are given in Table 1 parenthetically. One can see that the JISP16 interaction ensures a very fast convergence of the NCSM ab initio calculations. This is so for the calculations with the effective interaction, where the convergence is faster than for any other realistic interaction, and especially for the calculations with the bare interaction, in which case even a full-scale use of the potential of modern supercomputers in calculations involving very large model spaces usually proves to be insufficient for reaching convergence, so that the respective results are meaningless and cannot be a subject of a publication. In the case of the JISP16 interaction, the convergence rate for the bare interaction is somewhat lower than that for the effective interaction generated by JISP16, but it is comparable with the convergence rate for effective interactions generated by other realistic interactions. Ultimately, only for the JISP16 interaction can one find a confidence interval for the results of ab initio calculations, and this improves substantially the reliability of the results. In general, very narrow confidence intervals (those of width not larger than a few MeV units) were obtained for all nuclei studied here. For the light nuclei ^{3}H, ^{3}He, and ^{4}He, in which case the width of the confidence interval is about 0.1 MeV or even smaller, our results are highly reliable. The

Table 1. Binding energies of s- and p-shell nuclei according to NCSM calculations with the bare JISP16 interaction and with the effective interaction generated by the JISP16 interaction along with the NCSM model space and the $\hbar\omega$ values at which the results given here were calculated with the effective interaction (each number given parenthetically is the difference of the respective theoretical result and its counterpart obtained at the same value of $\hbar\omega$ in the nearest NCSM model space of smaller dimension)

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

confidence interval for the binding energy of the ^{10}B nucleus is as small as 0.56 MeV; it is 3 MeV for the ^{14}N nucleus, and so on. It is worth noting that the confidence interval becomes wider as the binding energy decreases in isobar chains. For example, the confidence interval is 3.2 MeV for the ^{13}C nucleus, but it is as wide as 9.9 MeV for the ^{13}O nucleus. Thus, the reliability of our results is lower for neutron-rich

and neutron-deficient nuclei, which are being vigorously studied at the present time. As was mentioned above, a confidence interval cannot be determined for $A = 6$–8 nuclei, in which case the calculations with the bare and the effective interaction are convergent on the same side. For these nuclei, we extrapolated the results to the case of an infinite model space, $N\hbar\omega \to \infty$, assuming that, in calculations with different values of the oscillator-basis parameter $\hbar\omega$, the binding energy converges exponentially to the same value as the size of the model space increases. For the ^{6}Li nucleus, the extrapolation of the binding energy calculated with the effective interaction leads to a value of 31.70(17) MeV (the value in parentheses is the estimated extrapolation error). A similar extrapolation for the ^{6}He nucleus yields 28.89(17) MeV. We emphasize that, for $A = 6$ nuclei, the results obtained with the bare and the effective interaction are very close: the binding energies calculated for ^{6}Li and ^{6}He with the bare interaction in the $12\hbar\omega$ model space are 30.94(44) and 28.23(41) MeV, respectively. The extrapolation of these calculations to $N\hbar\omega \to \infty$ leads to the binding energy of 31.33(12) MeV for ^{6}Li and the binding energy of 28.61(12) MeV for ^{6}He.

It is clear that JISP16, which is a realistic NN interaction, describes very well the binding energies of $A \leq 16$ nuclei. The experimental values of the binding energies for approximately half of these nuclei are within the confidence intervals of our predictions. However, the JISP16 interaction slightly underbinds nuclei in the middle of the p shell; the outliers beyond the boundaries of the confidence intervals of the binding energies for these nuclei are within a few percent, which corresponds to an unprecedented accuracy in the many-body nuclear problem. The binding energy proves to be underestimated for nuclei where the $p_{3/2}$ subshell is being filled; once the filling of this subshell has been completed and once the filling of the $p_{1/2}$ subshell has begun, the description of the binding energy is restored. Therefore, it is natural to assume that the JISP16 interaction generates a spin–orbit interaction of slightly underestimated strength in p-shell nuclei. The above discrepancy with the experimental data drops a hint as to how one can try to improve the JISP16 interaction. We emphasize that only within our approach, which is associated with constructing confidence intervals, do the flaws in the JISP16 interaction become obvious. In the customary NCSM approach and in other ab initio models, within which one only calculates binding energies with an effective interaction, nobody would pay attention to small deviations of the calculated binding energies from their experimental counterparts.

We emphasize that the values displayed in Table 1 do not result from a fit to the binding energies. Such a fit was constructed in smaller model spaces, and the description of the experimental situation was substantially better in that case. It is worth noting that, for all nuclei considered here, we have obtained correct values for the ground-state spin. Therefore, the many-body nuclear Hamiltonian based on the JISP16 NN interaction without three-nucleon forces appears to be a realistic Hamiltonian.

This conclusion is confirmed by the results of our calculations for the spectra and other properties of various nuclei—in particular, ^{6}Li and ^{10}B (see Tables 2 and 3). The choice of ^{6}Li and ^{10}B was motivated by the widespread opinion [6–10] that the spectra of these nuclei cannot be described without three-nucleon forces. In Tables 2 and 3, the results of our calculations are contrasted against the results obtained by other authors within various microscopic approaches involving the realistic Argonne NN potentials AV8′ and AV18 combined with various modern realistic three-nucleon forces [Tucson–Melbourne (TM′), Illinois (IL2), and Urbana (UIX)]. In addition, our results for ^{10}B are contrasted against the results of the NCSM calculations from [10], where use was made of the recently proposed realistic model ChPT relying on effective chiral field theory and including the two-nucleon interaction N3LO [11] (which was obtained in the fourth order of chiral perturbation theory, the parameters of this interaction being fitted to two-body NN data) and the three-nucleon interaction N2LO [12] (which was constructed in the third order of chiral perturbation theory). The bulk of the parameters of this three-nucleon interaction were taken from the two-nucleon interaction N3LO, while the remaining parameters were fitted in [10] to various properties of the ^{6}Li, ^{10}B and ^{12}C nuclei.

From Table 2, one can see that the description of the ^{6}Li nucleus on the basis of the JISP16 interaction compares well with the descriptions provided by interaction models that employ the best modern realistic two- and three-nucleon potentials. We note that, for the quadrupole moment of ^{6}Li, our approach yields a value very close to its experimental counterpart. It is well known that the ^{6}Li quadrupole moment is generated by subtle effects of the interference between the quadrupole moment of the deuteron cluster and the d-wave component of the relative motion of the clusters α and d. It should be noted that the value of $Q = -0.12\ e\ \mathrm{fm}^2$ was obtained in [10] for the ^{6}Li quadrupole moment on the basis of the ChPT interaction model. Unfortunately, the ^{6}Li spectrum was not presented in [10].

The energy spectrum of the ^{10}B nucleus is rather complicated, and it is difficult to reproduce this spectrum within a microscopic approach. The excitation

Table 2. Features of the ^{6}Li nucleus within various interaction models (our NCSM calculations were performed at $\hbar\omega = 17.5$ MeV): ground-state energy $E_{\text{g.s.}}$ and excitation energies in the E_x spectrum (in MeV units), root-mean-square charge radius r_p (in fm units), and ground-state quadrupole moment Q (in e fm^2 units)

Potential	Experiment	JISP16	AV8′ + TM′	AV18 + UIX	AV18 + IL2
Method		NCSM, $12\hbar\omega$	NCSM, $6\hbar\omega$ [6]	GFMC* [7, 8]	GFMC* [8, 13]
$E_{\text{g.s.}}(1^+_1, 0)$	−31.995	−31.00	−31.04	−31.25 (8)	−32.0 (1)
r_p	2.32 (3)	2.151	2.054	2.46 (2)	2.39 (1)
Q	−0.082 (2)	−0.0646	−0.025	−0.33 (18)	−0.32 (6)
$E_x(3^+, 0)$	2.186	2.529	2.471	2.8 (1)	2.2
$E_x(0^+, 1)$	3.563	3.701	3.886	3.94 (23)	3.4
$E_x(2^+, 0)$	4.312	5.001	5.010	4.0 (1)	4.2
$E_x(2^+, 1)$	5.366	6.266	6.482		5.5
$E_x(1^+_2, 0)$	5.65	6.573	7.621	5.1 (1)	5.6

* GFMC stands for the Green's function Monte Carlo method.

Table 3. Features of the ^{10}B nucleus within various interaction models and reduced probabilities of some $E2$ transitions (in e^2 fm^4 units) and Gamow–Teller transitions (our NCSM calculations were performed at $\hbar\omega = 15$ MeV; the notation is identical to that in Table 2)

Potential	Experiment	JISP16	AV8′ + TM′	AV18 + IL2	ChPT
Method		NCSM, $8\hbar\omega$	NCSM, $4\hbar\omega$ [6]	GFMC [9]	NCSM, $6\hbar\omega$* [10]
$E_{\text{g.s.}}(3^+_1, 0)$	−64.751	−60.14	−60.57	−65.6 (5)	−64.78
r_p	2.30 (12)	2.168	2.168	2.33 (1)	2.197
Q	+8.472 (56)	6.484	+5.682	+9.5 (2)	+6.327
$E_x(1^+_1, 0)$	0.718	0.555	0.340	0.9	0.523
$E_x(0^+, 1)$	1.740	1.202	1.259		1.279
$E_x(1^+_2, 0)$	2.154	2.379	1.216		1.432
$E_x(2^+_1, 0)$	3.587	3.721	2.775	3.9	3.178
$E_x(3^+_2, 0)$	4.774	6.162	5.971		6.729
$E_x(2^+_1, 1)$	5.164	5.049	5.182		5.315
$E_x(2^+_2, 0)$	5.92	5.548	3.987		4.835
$E_x(4^+, 0)$	6.025	5.775	5.229	5.6	5.960
$E_x(2^+_2, 1)$	7.478	7.776	7.491		7.823
$B(E2; 1^+_1 0 \to 3^+_1 0)$	4.13 (6)	3.317	1.959		3.05
$B(E2; 1^+_2 0 \to 3^+_1 0)$	1.71 (26)	0.627	1.010		0.50
$B(\text{GT}; 3^+_1 0 \to 2^+_1 1)$	0.083 (3)	0.042	0.066		0.07
$B(\text{GT}; 3^+_1 0 \to 2^+_2 1)$	0.95 (13)	1.652	1.291		1.22

* The numerical data for the excitation energies are due to J. Vary and P. Navrátil.

energies of ^{10}B depend greatly on the oscillator-basis parameter $\hbar\omega$. The dependence of the ground-state energy of ^{10}B on $\hbar\omega$ is weaker. In Table 3, we therefore give the results obtained at $\hbar\omega = 15$ MeV, which corresponds to the minimum energy of the first excited state, rather than at $\hbar\omega = 20$ MeV, which corresponds to the minimum of the $\hbar\omega$ dependence of the ground-state energy. So far, all microscopic calculations for the ^{10}B nucleus with realistic NN interactions have failed to describe even the ground-state spin without resorting to three-nucleon forces, to say nothing of the order of energy levels in the spectrum of this nucleus. In our calculations with the JISP16 two-nucleon interaction alone, we have obtained a very good description of the spectrum of ^{10}B. Not only have we been able to reproduce its ground-state spin, but we have also described the correct order of all levels in the spectrum, with the exception of the $(3_2^+, 0)$ state. We note that this state proved to be overly high in the spectrum not only in our calculations but also in the calculations performed in [6] with the Argonne NN potential AV8′ combined with the Tucson–Melbourne three-nucleon interaction TM′ and in the calculations performed in [10] on the basis of the chiral interaction model ChPT. We note that the ChPT interaction model also predicts an incorrect order of the $(2_1^+, 1)$ and $(2_2^+, 0)$ states, while the AV8′ + TM′ interaction model predicts incorrectly the order of a number of other levels. At the same time, Table 3 shows that not only does the JISP16 interaction provide a qualitative description of the ^{10}B spectrum, reproducing the correct order of the energy levels, but it also leads to a good quantitative description of the excitation energies. It is worth noting that the ^{10}B spectrum was not used in fitting the JISP16 interaction by means of phase-equivalent transformations.

It is also interesting to compare the predictions of various interaction models for electromagnetic and Gamow–Teller transitions. For all nuclei studied here, the JISP16 interaction provides a satisfactory description of these observables, which characterize the quality of the resulting many-body wave functions. For reasons of space, we illustrate this statement in Table 3 by presenting the reduced probabilities for only a few specific $E2$ and Gamow–Teller transitions. It is clear that our description of these quantities competes successfully with the results produced by other modern interaction models. In particular, our description of the reduced probabilities $B(E2; 1_1^+0 \to 3_1^+0)$ and $B(E2; 1_2^+0 \to 3_1^+0)$ is better than that within the ChPT interaction model. It should be emphasized that the parameters of the three-nucleon interaction in the ChPT model were fitted in [10] to data on the $E2$ transitions in question.

In conclusion, we have proposed a new approach of the *ab exitu* type in microscopic nuclear theory. This approach employs only experimental data on nuclear properties appearing as an ultimate output of microscopic calculations. Specifically, we begin by constructing NN interaction within the inverse-scattering approach on the basis of experimental data on deuteron properties and NN scattering, whereupon, in NCSM microscopic calculations, we perform a fine tuning of the NN interaction to the properties of s- and p-shell nuclei by means of phase-equivalent transformations. In constructing the JISP16 interaction, we do not use the ideas of meson-exchange theory, but by no means does this indicate that the resulting interaction is inconsistent with well-established facts that follow from the meson-exchange theories of nuclear forces. In particular, it is well known that, at comparatively long distances and in high-angular-momentum partial waves of NN scattering, the NN interaction is dominated by one-pion exchange. Both at long distances and in high-angular-momentum partial waves, the NN-scattering wave functions determined by the JISP16 interaction are virtually indistinguishable (see [3]) from the wave functions in the realistic Nijmegen NN potential, which is generated by the meson-exchange approach.

As a result, we have obtained a realistic multiparticle nuclear Hamiltonian based on the JISP16 NN interaction. This Hamiltonian is likely to give the best currently available description of the properties of s- and p-shell nuclei within a fully microscopic approach and, in addition, ensures a very fast convergence of NCSM calculations. As subsequent steps further along these lines, one can try to perform more accurate fits of the interaction parameters and to attain a still better description of the properties of light nuclei. In particular, we are going to construct a charge-symmetry-breaking interaction and to fit it independently to data on *np* and *pp* scattering. We expect that this interaction would make it possible to improve the description of many-body nuclear systems.

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