Recent shell-model investigation and its possible role in nuclear structure data study

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Abstract. Up to now, the nuclear shell model is rarely used in the nuclear data study because of several reasons. First, medium and heavy mass nuclei far from the shell-model cores, normally doubly magic nuclei, require a huge amount of calculation resource even in a limited shell-model space. Second, large deformation is difficult to be described in the limited model space, which is based on spherical symmetry. Third, high precision evaluation of nuclear structure data challenges the ability of the shell model. Even so, it is worth starting preliminary nuclear data investigations based on the shell model. With the present computational ability, it is possible to investigate 1000 or more nuclei in the framework of the shell model, which should be helpful for nuclear data study. In the present work, some recent shell-model investigations are briefly introduced. Based on these works, a simple nuclear force is suggested to be used in the systematic nuclear structure data study. The south-west region of ^{132}Sn is taken as an example to show the ability of such a simple nuclear force.

1 Introduction

Nuclear data is one of the key connections between nuclear physics and its application in many fields. For example, both the investigations on the nucleosynthesis in the universe and the chain reactions in the nuclear power plant require high precision nuclear data, such as nuclear structure data including masses, half-lives, levels, neutron separation energies, β decay properties, and ratios of delayed neutrons.

However, many nuclei involved in the nucleosynthesis and fission products in the reactor are beyond the present experimental abilities. Therefore, many nuclear structure data should be theoretically evaluated, such as the nuclear masses evaluated by the finite-range droplet model [1], the Hartree-Fock-Bogoliubov model [2], and the Weizsäcker-Skyrme mass model [3]. The nuclear shell model (SM) with configuration mixing is one of the most important models to understand the underlying physics of atomic nuclei [4, 5]. In SM, the eigenvalues (binding energies) and the eigenstates (wave functions) of both the ground and excited states are obtained simultaneously through the diagonalization process. The electromagnetic properties, β decays, and many other properties can be further calculated with the wave functions.

SM is used to understand the nuclear structure properties of the extreme neutron- and proton-rich nuclei observed in recent decades, but rarely used in the nuclear data study. One obvious reason is that the calculation cost of the nuclear shell model is vast, if the number of valence nucleons is large. Up to the present calculation limitation, around 10^{11} dimensions, it is possible to calculate 1000 or more nuclei through the shell model, which is much more than 20 years ago. It is worth performing systematic comparisons between the observed nuclear structure data and the shell-model results. If the structure properties mentioned above are well reproduced in the framework of the shell model, the further predictions on the unknown properties should be more reliable. Besides structure properties, SM can provide spectroscopic factors, which are important to cross section study [6, 7].

In the present work, some of our recent shell-model works will be firstly reviewed, including both the theoretical analysis and comparison with observations. Secondly, the south-west region of ^{132}Sn is taken as an example to show the ability of a simple nuclear force on the description of observed levels.

2 Recent Shell-model Study in Light, Medium, and Heavy Mass Nuclei

A Hamiltonian, YSOX, was suggested for *psd* region [8]. The neutron drip line of the B, C, N, and O isotopes are reproduced by YSOX but not by the previous Hamiltonians WBT and WBP [9]. ^{22}C was predicted to be rather weakly bound through YSOX and confirmed by the later experiment [11] and AME2012 [12]. The quadrupole deformation of ^{16}C is well described by YSOX [10]. The radius of two neutron halo nucleus, ^{22}C, was investigated based on the YSOX configuration and the neutron-neutron interaction [13]. In YSOX, the cross-shell interaction, especially its off-diagonal part, was reconsidered. It was shown that the levels, electromagnetic transitions, and B(GT) values of ^{14}C can be well described only with a $4\hbar\omega$ model space and a weaker off-diagonal interaction [14]. The recent observed neutron cross-shell properties of ^{11,12}Be are well reproduced by YSOX [15–17]. It is expected to investigate

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the island of inversion in *sdpf* region, with the northern boundary at ^{34}Si [18], through a similar method.

In *sd* region, phenomenological Hamiltonians, USD [19], USDA and USDB [20], are very successful, while realistic Hamiltonians can be obtained through *ab initio* method and V_{low-k} approach [21]. All three Hamiltonians in USD family are isospin symmetric without any mirror energy differences (MED), which are generally rather small. But some MED in nuclei around A= 20 are very large because of the weakly bound effect due to the protons in $1s_{1/2}$ orbit [22, 23]. With the inclusion of such effect in both single-particle energies and two-body matrix elements, the modified USD family can well describe MED in nuclei around A= 20 [23]. The recently measured β decay properties are well described through the modified Hamiltonian for ^{22}Si [24], ^{27}S [25, 26], and ^{26}P [27].

In the medium mass region, the nuclei around ^{132}Sn are especially important in nuclear data study due to their importance in both nucleosynthesis through *r*-process in the universe and the reactions in the reactor. For example, fission product yield has a peak in nuclei around A=140, of which the nuclear data contribute to the calculation of the present nuclear power plant [28]. The structure of ^{120,122}I, ^{140}Te, and ^{140}I were investigated recently, showing proton-neutron bands and isomers in ^{120,122}I [29, 30], the vibrator character of ^{140}Te [31], and the suppression of the B(GT) from ^{140}Te to ^{140}I [32]. In addition, the monopole effect is shown to be important for the description of core excitation and B(GT) in A = 130 nuclei [33].

A Hamiltonian was suggested for the south-east region of ^{132}Sn [34]. Based on the nice description of the observed neutron separation energies and levels, 8 isomers were predicted [34]. A later publication reported the first observation of spectroscopic property in this region, 2^+_1 state in ^{132}Cd with excitation energy 618(8) keV [35], while our Hamiltonian gives 710 keV. Recently, a new isomer was found in ^{134}In [36], which showed similar decay energy and transition strength to our prediction.

In the heavy mass region, the nuclear data of actinides are important for the transmutation of minor actinides in spent fuel [37] and the power distribution inside fuel rods of a thermal reactor [38–40]. It is impossible for SM to calculate all nuclei in this region at present, but the properties of nuclei close to ^{208}Pb can be well reproduced. For example, the ground state spin parity of ^{223}Np was observed with two possibilities, $9/2^-$ and $7/2^-$, while SM result supports the $9/2^-$ [41]. The isomeric state of ^{218}Pa is recently observed [42], but the spins and parities of the ground and isomeric states can not be experimentally determined with the present statistics. Different to the systematic trends of N= 127 isotones from ^{210}Bi to ^{216}Ac, which have 1^- ground states and high spin (8^- or 9^-) isomers, the ground and isomeric states of ^{218}Pa are suggested to be 8^- and 1^- states, respectively, based on SM results [42]. A new Hamiltonian for the south region of ^{208}Pb is under preparation, which described 45 observed binding energies within a root mean square (RMS) 0.09 MeV [43]. In addition, the neutron core excitation states of ^{209}Pb, ^{208}Pb, ^{207}Tl, and ^{206}Hg are well reproduced, which indicates the proper description of the N=126 gap.

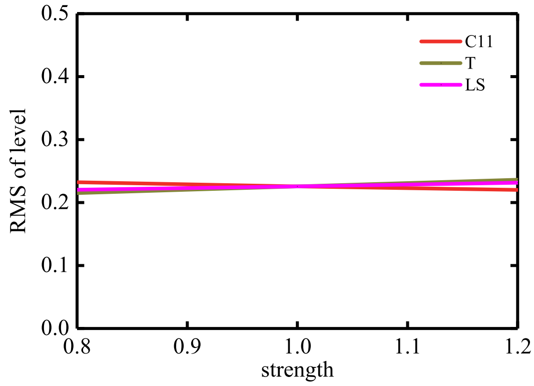

Figure 1. Root mean square of nearly 200 levels of isotopes and isotones of ^{132}Sn and ^{208}Sn as the function of strength of C11, LS1, and T1 terms

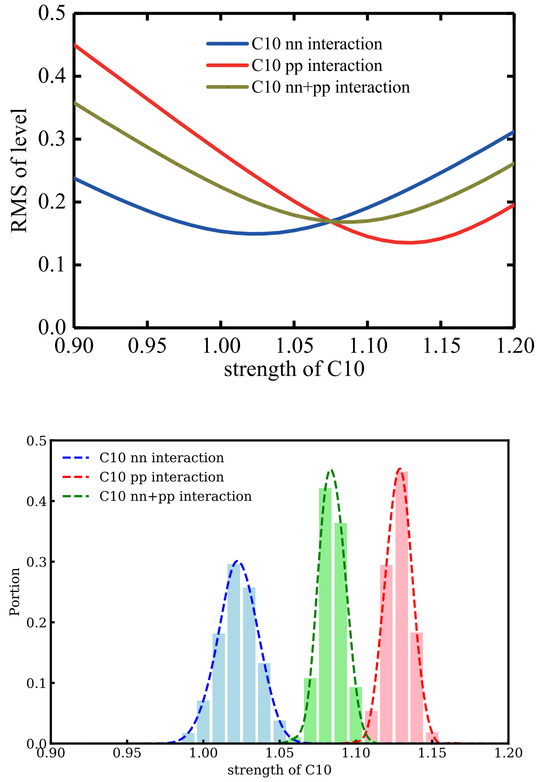

Figure 2. Upper panel: Root mean square of nearly 200 levels of isotopes and isotones of ^{132}Sn and ^{208}Sn as the function of strength of C10 term. Lower panel: Distribution of the strength of C10 term.

3 Applied V_{MU} to Nuclear Structure Data Study

Monopole based universal interaction, V_{MU}, is suggested through the monopole properties of central and tensor force [44]. V_{MU} plus spin-orbit interaction from M3Y

(V_{MU}+LS) is used as the cross-shell interaction in many regions, such as *psd* [8] and ^{132}Sn [34]. It is worth knowing the performance of the nuclear structure data purely from V_{MU}+LS. V_{MU}+LS includes 8 terms, central force with T=1, S=0 (C10), T=1, S=1 (C11), T=0, S=0 (C00), and T=0, S=1 (C01), spin-orbit force with T=1 (LS1) and T=0 (LS0), and tensor force with T=1 (T1) and T=0 (T0). If semi-magic nuclei are considered, only four T=1 terms contribute to the nuclear structure properties.

Considering nearly 200 levels in isotopes and isotones of ^{132}Sn and ^{208}Pb, it is found that a stronger strength of C10 is needed for proton-proton interaction comparing with that of neutron-neutron interaction [45]. Levels of ^{123,125}Ag are well reproduced through pure V_{MU}+LS with the strength for C10 term of proton-proton interaction 10% stronger than that of neutron-neutron interaction, which are 115% and 105% of the original strength, respectively [46]. The type II shell evolution is suggested in each neutron deficient In isotope from ^{101}In to ^{109}In based on SM calculations through such nuclear force with a little modifications [47]. In the present work, we further investigate the contribution of C11, LS1, and T1 terms. As seen in figure 1, the strengths of C11, LS1, and T1 change from 80% to 120% of their original values, but the RMS of levels are rarely affected by these three terms.

More detailed investigations on C10 term are also performed, as seen in the upper panel of figure 2. If the isotopes and isotones of ^{132}Sn and ^{208}Pb are considered together, around 107% of original C10 strength gives the minimum of RMS of levels at around 0.2 MeV. But if isotopes and isotones of ^{132}Sn and ^{208}Pb are separately considered, around 103% (113%) of original C10 strength gives the minimum of RMS of levels at around 0.15 (0.15) MeV for isotopes contributing by neutron-neutron interaction (isotones contributing by proton-proton interaction). With the bootstrap statistical method, the distribution of the strength is obtained, as seen in the lower panel of figure 2. It is clearly shown that the distribution of the strength for C10 term of proton-proton interaction has no overlap with that of neutron-neutron interaction. The strength of proton-proton interaction is statistically different from that of neutron-neutron interaction.

Table 1 and 2 present the SM results from V_{MU}+LS with different strengths for proton and neutron parts. Observed data and results from jj45pna and jj45pnm are also presented. Nuclei in the south-west region of ^{132}Sn with observed levels and $A \geq 126$ are considered as examples. jj45pna is from G matrix calculation and included in OXBASH package [48]. jj45pnm is modified version of jj45pna with 77% (92%) of proton-proton (neutron-neutron) interaction. Such modifications give a better description on levels of nuclei around ^{132}Sn. Single-particle energies of the three Hamiltonians are taken to be the same as the observed levels of ^{131}Sn and ^{131}In.

Comparing with 88 levels in 15 nuclei, the RMS of levels are 0.17, 0.27, and 0.47 for V_{MU}+LS, jj45pnm, and jj45pna, respectively, as shown in table 3. Simple nuclear force V_{MU}+LS gives a very nice description of the observed levels. Considering the RMS of individual nucleus, V_{MU}+LS provides rather stable descriptions without very

Table 1. Observed and calculated levels of $^{126-130}$Sn and $^{127-130}$In. Observed data are taken from NNDC [49].

nucleus	Jπ	Expt.	V_{MU}+LS	jj45pnm	jj45pna
^{126}Sn	0+	0.00	0.00	0.00	0.00
	2+	1.14	1.31	1.15	1.27
	4+	2.05	1.92	2.06	2.28
	5-	2.16	2.13	2.25	2.49
	7-	2.22	2.12	2.32	2.57
	6-	2.48	2.19	2.49	2.76
	(8+)	2.49	2.20	2.51	2.78
	(10+)	2.56	2.26	2.54	2.81
^{127}Sn	11/2-	0.00	0.00	0.00	0.00
	3/2+	0.01	0.05	0.03	0.04
	(1/2)+	0.26	0.19	0.18	0.19
	(9/2)-	0.65	0.93	0.76	0.85
	(5/2+)	0.81	1.04	0.91	1.01
	(7/2-)	0.96	1.14	0.88	0.96
	(7/2+)	1.05	1.24	1.29	1.43
	(15/2-)	1.09	1.24	1.04	1.15
^{128}Sn	0+	0.00	0.00	0.00	0.00
	(2)+	1.17	1.31	1.23	1.36
	(4+)	2.00	1.87	2.03	2.24
	(7-)	2.09	1.99	2.14	2.37
	(5-)	2.12	2.03	2.17	2.40
^{129}Sn	3/2+	0.00	0.00	0.00	0.00
	11/2-	0.04	0.01	0.05	0.05
	(1/2)+	0.32	0.23	0.31	0.32
	(9/2-)	0.76	1.00	1.14	1.24
	(5/2+)	0.77	0.95	0.96	1.06
	(7/2-)	1.04	1.16	1.04	1.13
	(7/2+)	1.05	1.16	1.21	1.34
	(15/2-)	1.17	1.27	1.24	1.35
^{130}Sn	0+	0.00	0.00	0.00	0.00
	(2+)	1.22	1.33	1.42	1.56
	(7-)	1.95	1.86	1.92	2.13
	(4+)	2.00	1.85	2.13	2.35
	(5-)	2.08	1.96	2.08	2.30
	(4-)	2.21	1.85	2.17	2.41
	(6+)	2.26	2.01	2.34	2.58
	(8+)	2.34	2.08	2.42	2.67
	(10+)	2.43	2.16	2.48	2.73
^{127}In	(9/2+)	0.00	0.00	0.00	0.00
	(1/2-)	0.41	0.05	0.04	0.03
	(3/2-)	0.93	0.62	0.37	0.38
	(21/2-)	1.86	1.88	1.99	2.22
^{128}In	(3)+	0.00	0.00	0.00	0.00
	(1-)	0.25	0.06	0.32	0.29
	(8-)	0.34	0.65	1.05	1.06
	1+	1.17	0.97	0.65	0.66
^{129}In	(9/2+)	0.00	0.00	0.00	0.00
	(1/2-)	0.46	0.21	0.16	0.15
	(11/2+)	1.00	1.07	1.33	1.46
	(3/2-)	1.09	0.87	0.65	0.67
	(13/2+)	1.35	1.28	1.34	1.45
	(5/2+)	1.42	1.57	1.49	1.58
^{130}In	1(-)	0.00	0.00	0.00	0.00
	(10-)	0.05	0.35	0.28	0.28
	(3+)	0.39	0.40	0.46	0.46
	(5+)	0.40	0.59	0.56	0.57
	1+	2.12	1.79	1.38	1.44

Table 2. The same as table 1 but for $^{126,128-130}$Cd and ^{126,128}Pd.

nucleus	Jπ	Expt.	V_{MU}+LS	jj45pnm	jj45pna
^{126}Cd	0+	0.00	0.00	0.00	0.00
	(2+)	0.65	0.91	0.78	0.90
	(4+)	1.47	1.73	1.68	1.90
^{128}Cd	0+	0.00	0.00	0.00	0.00
	(2+)	0.65	0.90	0.95	1.13
	(4+)	1.43	1.65	1.91	2.21
	(5-)	1.87	1.87	1.86	2.19
	(7-)	2.11	1.97	2.20	2.44
	(6+)	2.20	2.18	2.75	3.14
	(8+)	2.65	2.48	3.18	3.63
	(10+)	2.71	2.55	3.40	3.63
^{129}Cd	11/2-	0.00	0.00	0.00	0.00
	(13/2-)	1.18	1.22	1.44	1.86
	(15/2-)	1.59	1.60	1.82	2.20
	(21/2+)	1.94	2.11	2.05	2.53
^{130}Cd	0+	0.00	0.00	0.00	0.00
	(2+)	1.33	1.34	1.40	1.96
	(4+)	1.86	1.81	1.93	2.71
	(6+)	1.99	1.97	2.11	2.96
	(8+)	2.13	2.08	2.22	3.10
^{126}Pd	0+	0.00	0.00	0.00	0.00
	(2+)	0.69	0.98	0.82	1.05
	(4+)	1.48	1.83	1.66	2.07
	(5-)	2.02	2.03	2.09	2.54
	(7-)	2.11	1.98	2.26	2.55
	(10+)	2.41	2.61	3.73	3.80
^{128}Pd	0+	0.00	0.00	0.00	0.00
	(2+)	1.31	1.41	1.46	2.03
	(4+)	1.82	1.90	2.01	2.83
	(6+)	2.08	2.08	2.20	3.09
	(8+)	2.15	2.18	2.30	3.22

Table 3. Root mean square between observed data and calculations for each nucleus and all nuclei in tables 1 and 2.

nucleus	V_{MU}+LS	jj45pnm	jj45pna
^{126}Sn	0.20	0.05	0.26
^{127}Sn	0.17	0.11	0.17
^{128}Sn	0.10	0.04	0.22
^{129}Sn	0.13	0.16	0.23
^{130}Sn	0.21	0.09	0.27
^{127}In	0.24	0.34	0.38
^{128}In	0.21	0.44	0.44
^{129}In	0.16	0.26	0.29
^{130}In	0.22	0.35	0.33
^{126}Cd	0.21	0.14	0.29
^{128}Cd	0.15	0.42	0.68
^{129}Cd	0.09	0.18	0.54
^{130}Cd	0.04	0.08	0.77
^{126}Pd	0.21	0.55	0.69
^{128}Pd	0.06	0.14	0.86
total	0.17	0.27	0.47

large RMS in each nucleus. But for jj45pnm and jj45pna, nuclei with strong proton and neutron configuration mixing are poorly described, such as for ^{128}In, ^{128}Cd, and ^{126}Pd. Even though further and more systematic investigation should be carefully performed, the present results show the possibility of applying V_{MU} to nuclear structure data study. The uncertainty of such a theoretical description also needs to be taken into account through statistical methods, such as the uncertainty decomposition method [50] and the bootstrap statistical method [51]. The uncertainties of the observed data are also not included in the present fitting, which should be considered if they are as large as the theoretical ones (around 0.1 MeV).

4 Conclusion

Based on some recent shell-model investigations, a simple nuclear force, V_{MU}+LS is suggested to be applied to nuclear structure data study. As an example, levels of nuclei in the south-west region of ^{132}Sn are investigated. It is shown that V_{MU}+LS can give very nice descriptions of the observed levels, with 0.17 MeV RMS. It is worth to perform systematic investigations on the medium and heavy mass region to see the performance of V_{MU}+LS on the binding energies, levels, electromagnetic transitions, and many other properties.

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