Effective interaction for nuclei of A=50-100 and Gamow-Teller properties

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Abstract. A new effective interaction is proposed for shell-model calculations in the model space consisting of single-particle orbits $p_{3/2}$, $f_{5/2}$, $p_{1/2}$, and $g_{9/2}$. Starting from a realistic interaction derived from the nucleon-nucleon potential, Hamiltonian parameters are modified by a least-squares fit to experimental energy data. The resultant interaction JUL32 is tested from various viewpoints. The property of Gamow-Teller transition strength is studied in the full pf-shell model space focusing on nuclei around 56 Ni, where the shell-model results show significant dependence on the choice of the effective interaction.

1. Introduction

The Monte Carlo shell model [1] (MCSM) has enabled us to apply the nuclear shell model to various problems such as the shell-evolution in neutron-rich nuclei and the shape coexistence, which require explicit treatment of a huge model space and many valence nucleons and therefore have not been accessible by conventional diagonalization methods. On the other hand, the effective interaction for practical use in such a huge model space is in many cases not well-known. We have been investigating a possibility to construct an effective interaction which can be used in a complete $0\hbar\omega$ space and beyond it with a reasonable predictive power, and have published a possible solution GXPF1 [2, 3] for pf-shell nuclei.

In this paper, we first discuss our recent trial to describe heavier nuclei around A=60-100 in the shell-model framework and propose a new effective interaction. A reasonable choice of the model space is to include the single-particle orbits $p_{3/2}$, $f_{5/2}$, $p_{1/2}$ and $g_{9/2}$, taking ⁵⁶Ni as an inert core. Hereafter, we call this model space f_5pg_9 -shell. One advantage of this choice is that this model space is free from the spurious center of mass motion. The largest M-scheme dimension of this model space reaches about 13 billions, which is beyond the current basis-size limitation in the conventional diagonalization method, and the MCSM can play a role.

The spin-isospin response is one characteristic property of the nuclear system, and has been a crucial test of the nuclear structure models and calculations. The Gamow-Teller strength distribution of nuclei in the middle of the pf-shell is of special importance from astrophysical viewpoints. Recent high-resolution data can be compared to the shell-model results not only as a gross distribution but also as individual strengths. Therefore, as the second topic, we present several shell-model results with the GXPF1 interaction (and its modified version), focusing especially on nuclei around 56 Ni, where this interaction has been confirmed to be quite successful. The results are compared to those of other interactions in order to show to what extent the shell-model prediction depends on the choice of the effective interaction.

2. Effective interaction for f5pg9-shell nuclei

The effective interaction can in principle be derived in a microscopic way from a realistic nucleonnucleon potential. However, such an interaction is not necessarily successful in describing experimental data especially for cases with many valence nucleons. One possible way to overcome this problem is to modify such an interaction by fitting to experimental data, as demonstrated in the cases of the p-shell [4], sd-shell [5], and also pf-shell [2, 3]. We follow the same line.

Special care should be taken in the choice of the experimental data to be fitted. First of all, the 56 Ni core is relatively "soft" [3, 6] and the excitation from the $f_{7/2}$ to other orbits is significant in Ni isotopes. Therefore we exclude all Ni isotopes from the fit. In addition, for many nuclei in the middle of the present model space, very large B(E2) values are observed experimentally for transitions among low-lying states, suggesting large deformation. We found that the present model space is insufficient to describe such a large quadrupole collectivity because of the lack of the $d_{5/2}$ orbit. Therefore, we also exclude the data of nuclei with N < 46 and Z > 33. In order to keep the number of data minimal, we take mainly even-Z nuclei (the exceptions are 65,67,69,71 Cu and the N = 50 isotones 85 Br, 87 Rb, 89 Y, 91 Nb, 93 Tc and 95 Rh). In total, we take 310 experimental binding and excitation energy data out of 69 nuclei with A=63-96.

As a starting Hamiltonian, we take a microscopic interaction [7] derived from the Bonn-C potential, which is denoted by G-f5pg9. The same type of an interaction [8] was used in the derivation of the GXPF1. Details of iterative fitting methods and adopted approximations in the shell-model calculations are described in Ref.[9]. Assuming the isospin symmetry, the shell-model Hamiltonian is specified by 133 two-body matrix elements and four single-particle energies. In the latest step of the iteration, we have varied 32 well-determined linear combinations of these parameters. A common mass dependence factor $A^{-0.3}$ is assumed for all two-body matrix elements. We have attained the rms error of 213 keV with the resultant interaction, JUL32.

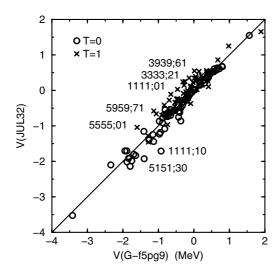
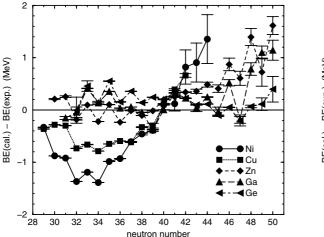


Figure 1. Comparison of two-body matrix elements V(abcd; JT) between the G-f5pg9 and the JUL32. Labels $2j_a2j_b2j_c2j_d; JT$ are shown explicitly for several matrix elements.



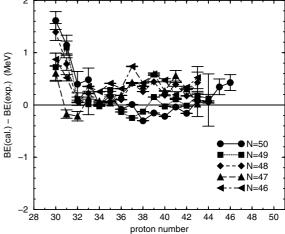
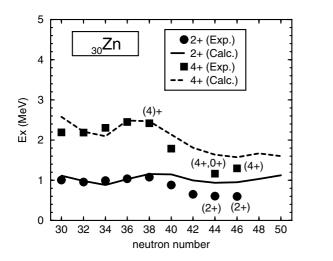


Figure 2. Difference between the experimental and the calculated binding energies. The left (right) panel shows the results of $28 \le Z \le 32$ isotopes ($46 \le N \le 50$ isotones) as a function of the neutron (proton) number. Experimental data are taken from Ref.[11]

In Fig.1, one can find reasonable correlation between two-body matrix elements of the starting G-f5pg9 Hamiltonian and that of the fitted one JUL32. The T=0 (T=1) matrix elements are, in average, modified to be more attractive (repulsive) by the fit. In addition, relatively large changes can be found mainly in diagonal matrix elements V(abab; JT) with large J, and also in monopole-pairing ones V(aabb; 01). We have obtained the same general observations in the case of the pf-shell [3].

Binding energies are evaluated by taking into account the Coulomb energies according to the empirical formula [10] $E_C(\pi,\nu) = \pi \varepsilon_C + \frac{1}{2}\pi(\pi-1)V_C + [\frac{1}{2}\pi]b_C + \pi \nu \Delta_{np}$, where π (ν) stands for the number of valence protons (neutrons). We use the parameter set 2 in TABLE I of Ref.[10] for values of ε_C , V_C , b_C and Δ_{np} . The difference between experimental binding energies and the shell-model results are shown in Fig.2. It can be seen that the agreement is reasonable for $Z \geq 32$. The largest discrepancy is found in Ni isotopes, partly because no data of Ni isotopes was include in the fit. The shell-model prediction is underbinding for N < 40 and overbinding for N > 40, which can be understood by considering the effects of the missing $f_{7/2}$ orbit in the present model space. Since the T=0 monopole attraction between the $\pi f_{7/2}$ and $\nu f_{5/2}$ [12] is much stronger than that of the $\pi f_{7/2}$ and $\nu g_{9/2}$, if the $f_{7/2}$ orbit is included, it should relatively enhance the binding for N < 40 and reduce for N > 40. The similar but somewhat weaker effect can be found also in Cu isotopes.

Low-lying energy spectra of even-even nuclei show characteristic behavior depending on the nuclear structure, and the description of their systematics can be a good test of the effective interaction. In Fig.3, excitation energies of the yrast 2^+ and 4^+ states are plotted for Zn isotopes and N=48 isotones. In the case of Zn isotopes, the description is successful for N<40, while systematic discrepancies exist for $N\geq 40$, i.e., the shell-model fails to reproduce the sudden decrease of the excitation energies, suggesting insufficient quadrupole collectivity. We have found the similar problem also in Ge and Ni isotopes, which can again be traced back to the lack of the $f_{7/2}$ orbit. Considering the strong repulsion between the proton $f_{7/2}$ and the neutron $g_{9/2}$ orbit due to the tensor interaction [13], the effective single-particle energy of the proton $f_{7/2}$ orbit raises relative to the upper orbits. Thus proton excitations should become important beyond N=40. On the other hand, the agreement between the data and the shell-model prediction is quite good for N=48 isotones over the whole range of the proton number.



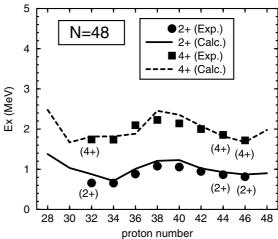


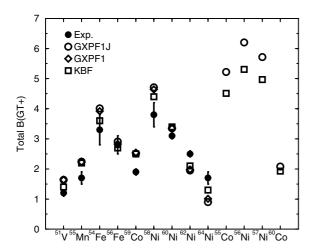
Figure 3. Energy levels of low-lying states. The left (right) panel shows the results of Zn isotopes (N=48 isotones) as a function of the neutron (proton) number. Experimental data are taken from Ref.[14]

3. Gamow-Teller properties around ⁵⁶Ni

We first consider the M1 distribution in order to calibrate the spin-flip strength in the effective interaction. We start with the latest version GXPF1A [15], which gives improved description for neutron-rich Ca, Ti, Cr isotopes. It is known experimentally that, in ⁴⁸Ca, most of the M1 strength is concentrated in only one state at 10.23 MeV [16]. The GXPF1A predicts 83% of the total strength at 10.90 MeV. We multiply the multipole part of the two-body matrix elements $V(f_{7/2} f_{5/2} f_{7/2} f_{5/2}; J1)$ by a common factor 0.7 for all J, so that the resultant interaction, GXPF1J, reproduces the experimental excitation energy. The total M1 strength 10.8 μ_N^2 is almost unchanged by this modification. By introducing the same spin-quenching factor q=0.74 as deduced in Ref. [17], we obtain a summed strength 5.8 μ_N^2 in an excitation energy range E_x =8-13MeV, which is consistent with the experimental data 5.3(6) μ_N^2 [18].

In Fig.4, the total GT+ strengths are shown for various nuclei. The shell-model results are obtained with three different effective interactions, GXPF1J, GXPF1 and KBF [19]. A common quenching factor q=0.74 is taken for comparison. It can be seen that the experimental data are reasonably well reproduced by all these interactions. The difference between the GXPF1 and the GXPF1J is rather small. On the other hand, the difference between the KBF and the GXPF1J becomes large in 56 Ni, 57 Ni and 55 Co, which reflects the difference in the description of core-excitations between these two interactions. In fact, the KBF interaction predicts higher excitation energies than the GXPF1 by about 0.8MeV for low-lying states such as $11/2_1^-$ in 55 Co and 2_1^+ in 56 Ni, which are composed mainly of $f_{7/2}$ -core excited configurations. Such differences around 56 Ni can be found also in the excitation energies of the centroids (see the left panel). We have carried out the similar comparison between these two interactions for the GT- direction. The centroid energies predicted by the GXPF1J are systematically higher than those of the KBF by about 2 MeV for Ni isotopes. Since the KBF interaction has been extensively used for astrophysical calculations [24], it is interesting to study whether this difference can give some impact on the astrophysical predictions.

In addition to the total strength, it is interesting to compare individual strengths obtained by recent high-resolution experiments with the shell-model prediction. As an example, in Fig.5, the GT- strengths in ⁵⁸Ni are shown. One can find significant difference between two shell-model results obtained with the GXPF1J and the KB3G [25] interaction. The GXPF1J successfully



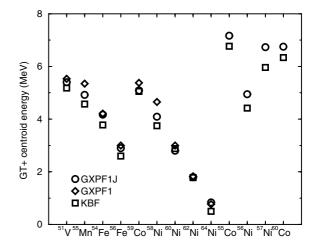


Figure 4. Properties of GT+ transitions. In the left panel, experimental data of the total GT+ strengths are compared with the shell-model predictions. Experimental data are taken from Refs. [20, 21, 22, 23]. The right panel shows the corresponding centroid energies.

describes the excitation energies of the lowest two peaks as well as the structure around 3.5 MeV. However, the absolute strength of the second peak is underestimated. On the other hand, the KB3G interaction reproduces the relative height of the first and the second peaks, while their absolute strengths are overestimated. In addition, the structure around 3.5 MeV is missing. In order to understand the origin of these differences between the two shell-model results, it is useful to decompose each strength into the contribution of the p-orbit and the f-orbit. We have found that the lowest two peaks consist mainly of the p-orbit contribution. In the lowest peak (58 Cu ground state), the f-orbit contribution is also large with the opposite sign relative to the p-orbit one, and the cancellation is significant. Among the f-orbit components, the GXPF1 predicts larger contribution of the spin-flip $\nu f_{7/2} \to \pi f_{5/2}$ transition than that of the KB3G. Therefore the destructive f-orbit contribution is relatively larger in the GXPF1J, which reduces the GTstrength of the lowest state. In the results of the GXPF1J, several peaks around 3.5 MeV consist mainly of the f-orbit contribution, corresponding to various core-excited configurations. Such f-dominant peaks can be found around 5 MeV in the results of the KB3G. Thus the absolute strength is very sensitive to the configuration mixing in the wave functions, which reflects the property of the effective interaction.

4. Summary

A new effective interaction JUL32 has been proposed for practical use in the f_5pg_9 -model space, which reasonably describes binding energies and low-lying energy spectra over a wide mass range within the present model space. Clear effects of the missing $f_{7/2}$ orbit can be seen, for example, in the $E_x(2_1^+)$ systematics of Zn isotopes for N > 40. Our next step is to extend further the model space by taking into account the neighboring orbits such as the $f_{7/2}$ and the $d_{5/2}$, which will enable us to study the variation of nuclear structure along the N = Z line, including large deformation and the shape coexistence.

It has been shown that the shell-model prediction of the Gamow-Teller strength distribution is sensitive to the choice of the effective interaction especially around ⁵⁶Ni. Our interaction GXPF1 predicts somewhat different results in comparison to the existing ones, which may have some impact on astrophysical scenarios such as the supernovae explosion. Detailed comparison between the recent high-resolution data and the shell-model prediction provide us precious information on the effective interaction.

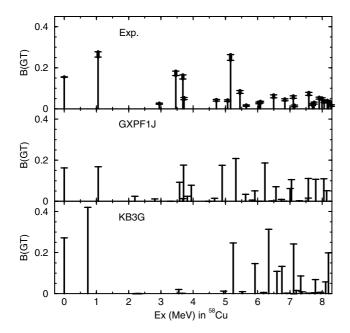


Figure 5. The GT- strength distribution in 58 Ni. The top panel shows the experimental data [26], while the shell-model prediction by the GXPF1J (KB3G) interaction is presented in the middle (bottom) panel. The shell-model results are obtained by using the code MSHELL [27], allowing at most 5 nucleons to excite from the $f_{7/2}$ orbit to upper orbits. States up to around 5 MeV are almost converged eigenstates after 100 Lanczos iterations for each isospin. A common quenching factor q=0.74 is used for both interactions.

Acknowledgments

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