Effective interaction for f5pg9-shell nuclei and two-neutrino double beta-decay matrix elements

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Abstract. We have developed an effective interaction for shell model calculations in the model space consisting of four orbits 1p3/2, 0f5/2, 1p1/2 and 0g9/2. Starting from a renormalized G-matrix interaction, we have modified 45 linear combinations of Hamiltonian parameters by fitting to 400 experimental binding and excitation energy data out of 87 nuclei with masses A=63-96. The resultant effective interaction is shown to be successful for describing irregular behavior of the 02+ states in Ge isotopes. We have evaluated the two-neutrino double-beta-decay matrix elements for 76Ge and 82Se which are in reasonable agreement with the experimental data.

1. Introduction

The effective interaction is a key ingredient for successful shell-model calculations. Owing to recent developments in computational facilities as well as novel techniques of numerical calculations such as the Monte Carlo shell model [1], the applicability of the shell model is rapidly expanding. On the other hand, our knowledge of the effective interaction is still insufficient especially for cases where more than one major shell should be included in an active valence space. Such a treatment is essentially important for describing neutron-rich nuclei.

We have developed a new effective interaction for shell-model calculations in the model space consisting of valence orbits 1p3/2, 0f5/2, 1p1/2 and 0g9/2 assuming an inert 56Ni core. This space is called f5pg9-shell, hereafter. It can be regarded as a first step for future extensions to the pf+sdg model space. We have carried out the similar iterative fitting calculations as in the case of the pf-shell [2, 3]. Starting from a microscopic interaction (renormalized G-matrix) [4, 5] based on a realistic NN-potential, we have varied 45 linear combinations of Hamiltonian parameters (133 two-body matrix elements and four single-particle energies) by a least-squares fit to the 400 experimental binding and excitation energy data out of 87 nuclei with masses A=63-96. The quality of the fit has been improved in comparison with our previous results [6]. In the latest iteration, we have attained the rms error of 185 keV.

In this paper, we present two applications of this interaction. In section 2, we discuss the systematic behavior of the low-lying states in Ge isotopes. In section 3, the double beta-decay
is considered for $^{76}\text{Ge}$ and $^{82}\text{Se}$, focusing on the two-neutrino mode. Shell-model calculations have been carried out in a conventional way by using the code MSHELL. [7]

2. Low-lying states in Ge isotopes

It has been argued that there exists significant change of structure between the lighter ($N < 40$) and heavier ($N > 40$) Ge isotopes, which can be interpreted as a phase transition from the spherical (or oblate) to prolate shape [8] and also the coexistence of them. Such a change can be seen in various experimental observables such as the nucleon transfer cross sections [9] and $B(E2)$ values and their ratios of low-lying states [10]. The behavior of the $0^+_2$ state is especially interesting from the viewpoint of the shell-model description including the “intruder” configuration. As a function of $N$, the excitation energy of the $0^+_2$ state decreases rapidly and reaches the minimum at $N = 40$, which corresponds to the first excited state of $^{72}\text{Ge}$. Experimental $B(E2)$ data suggest that there is no deformed band on top of this state, but it can be an “intruder” state with spherical shape [11]. There have been many theoretical approaches to this problem such as the boson expansion techniques [12], the interacting boson model [13] and the Hartree-Fock-Bogoliubov method with the quantum number projection [14], which are based on the mean-field picture or the collective model. Thus it is quite interesting to apply the microscopic shell-model because it is suitable to describe detailed structure in such a transitional region, including the neighboring odd-mass nuclei within a common framework.

Figure 1 shows the energy levels of low-lying states for even-$A$ (left panel) and odd-$A$ (right panel) Ge isotopes. It can be seen that the shell-model results reasonably reproduce the experimental data. Especially, the irregular behavior of the $0^+_2$ states around $N = 40$ is successfully described. In order to understand the structure of these states, the occupation number of the neutron $g_{9/2}$ orbit is shown in fig.2. It looks very similar for the $0^+_1$ and the $2^+_1$ states, suggesting the same intrinsic structure which varies smoothly as a function of $N$. According to a naive filling configuration, this number is expected to be 0 for $N \leq 40$ and $N - 40$ for $N > 40$. However, in the shell-model wave function, because of the deformation and the pairing effect, additional neutrons are excited to the $g_{9/2}$ orbit. The number of such additional neutrons increases toward the middle of the model space, and reaches the largest value of about 3 at $N = 40$. There is no shell-model configuration which dominate the wave functions of these states, and they can be interpreted as collective deformed states. On the
other hand, the occupation number of the 0\(^+\) state shows quite different \(N\) dependence for \(36 \leq N \leq 44\). It is close to 2 for \(N \leq 40\) and \(N - 38\) for \(N > 40\), which is consistent with the picture of two-neutron excitation from the pf-shell to the \(g_{9/2}\) orbit on top of the filling configuration. As for the \(^{72}\text{Ge}\), the wave function of the 0\(^+\) state is dominated by the closed shell configuration \(\pi(p_{3/2})^4(\nu(p_{3/2})^4(f_{5/2})^6(p_{1/2})^2\) with the probability of 37\%, which suggests a nearly spherical shape. Thus, our shell-model result support the picture of the spherically-deformed shape coexistence in \(^{72}\text{Ge}\).

Although the shell-model results reasonably reproduce the energy levels of yrast states and the systematics of the 0\(^+\) state, we find several difficulties mainly in the quantitative description of collective properties, which can naturally be attributed to the insufficiency of the model space. For example, as shown in fig. 3, the value of \(B(E2; 0^+ \rightarrow 2^+)\) is predicted to be larger for \(N < 40\) and smaller for \(N=42, 44\) than the experimental data. Another example is the quadrupole moment of the 2\(^+\) state. Experimentally, it changes the sign from \(N = 40\) to 42 as shown in table 1, which indicates the shape transition from the oblate (spherical) to prolate shape. On the other hand, in the shell-model results, the change of the sign is also found, but its position is shifted to around \(N = 46\). This reslt suggests the insufficiency of the quadrupole collectivity which favours the prolate deformation. The \(f_{7/2}\) orbit is missing in the present model space, which is important to generate such prolate deformation. The excitation from the proton \(f_{7/2}\) orbit becomes important especially when neutrons begin to occupy the \(g_{9/2}\) orbit, because the strong repulsive force between the proton \(f_{7/2}\) and the neutron \(g_{9/2}\) orbit should lead to
narrower $Z = 28$ shell gap \[17\]. Thus it is interesting problem to extend the model space by including the $f_{7/2}$ orbit, which is definitely needed to investigate more neutron-rich cases.

3. Double beta-decay matrix elements

As another application of the new effective interaction, we try to evaluate the nuclear matrix element of the double $\beta$-decay for $^{76}$Ge and $^{82}$Se, focusing on the two-neutrino mode. For these nuclei the double $\beta$-decay lifetime has been measured experimentally, which is related to the nuclear matrix elements as

$$
[T_{1/2}^{(2\nu)}(0^+ \rightarrow 0^+)]^{-1} = G \left | M_{GT}^{(2\nu)} \right |^2,
$$

where $G$ denotes a phase space factor including the weak-coupling constant. We can compare the experimental values with our shell-model results, which are calculated according to the following expression

$$
M_{GT}^{(2\nu)} = \sum_{m} \langle 0_f^+ || \sum_{k} \sigma_k \tau_k^- || 1_i^+ \rangle \langle 1_i^+ || \sum_{k} \sigma_k \tau_k^- || 0_f^+ \rangle \frac{1}{2} Q_{\beta\beta} + E_{x}(1_i^+) - E_0,
$$

where $E_0$ stands for the mass difference between the parent and intermediate nuclei. Since the nuclear matrix element $M_{GT}^{(2\nu)}$ depends on both the initial and the final state wave functions as well as the Gamow-Teller strength distribution in the intermediate states, it provides us with a stringent test of the theoretical model.

In usual shell-model calculations for the Gamow-Teller matrix elements within a restricted model space, we need to “quench” the spin operator in order to obtain reasonable comparison with the experimental data. Specifically, the Gamow-Teller operator $T(GT-) = \sum_{k} \sigma_k \tau_k^- \tau_{k'}^+$ is multiplied by a quenching factor $q$. The amount of the quenching should be taken consistently with the systematics over the nuclei described within the adopted model space. One can find a standard value of this factor in the literature: $q=0.82$ for the p-shell \[18\], 0.77 for the sd-shell \[19\] and 0.74 for the pf-shell \[20\] space, respectively. Thus we first estimate a suitable quenching factor in the present $f_{5/2}g_{9/2}$-shell. For this purpose, we try to fit as many experimental data as possible for known Gamow-Teller $\beta$-decay among low-lying states by using a common quenching factor. It should be noted that, in the present $f_{5/2}g_{9/2}$-shell, the Ikeda sum-rule $S_- - S_+ = 3(N - Z)$ is violated because the spin-orbit partner for the $f_{7/2}$ orbit and the $g_{9/2}$ orbit is missing in the model space. As far as we consider transitions among low-lying states, the spin-flip transitions may not be important and then this problem should not be serious. This restriction of the validity to the low-lying states can be justified to some extent for the evaluation of the two-neutrino mode because of the energy denominator in eq.(2).

For each low-lying transition, we extract the effective Gamow-Teller matrix element from the experimental $B(GT)$ value as $M_{GT} = \sqrt{(2J_i + 1)} B(GT)$, and compare it with the corresponding shell-model result. Here, experimental $B(GT)$ values are derived from the log $ft$ data in ref. \[15\]. In the left panel of fig.4 we summarize such a comparison. We classify the available data into three sets A, B and C according to the reliability. The set A contains all available data including the states where the spin assignment is not necessarily certain, and the set B includes the data with a firm spin assignment, and the set C includes the data which are selected from the set B under the criterion that the difference in the excitation energy between the experimental value and the corresponding shell model result is less than 0.1 MeV for both the initial and the final states. As expected, it is difficult to draw a definite conclusion form the results of set A, while for the set C, one can find a certain correlation between the data and the calculation. We obtain the value $q = 0.53$ from a least-squares fit by using the set C, although the uncertainty is rather large.

In order to reduce the uncertainty due to a possible failure in the shell-model description of detailed mixing among low-lying states, we next consider the total strength summed over the
Figure 4. Correlations between the experimental data and the shell-model results for the individual effective Gamow-Teller transition matrix elements (left panel) and the normalized strength summed over the final states (right panel). Data are taken from ref.[15].

all final states and normalized it by the sum-rule value. For each initial state, we evaluate the value $T = \sqrt{\sum_f M_{if}(i \rightarrow f)^2/W}$, where the normalization factor is calculated for the parent nucleus as $W = |g_A/g_V|\sqrt{(2J_i+1)3|N_i-Z_i|}$. (If $N_i = Z_i$, we use the daughter nucleus.) The comparison between the data and the calculation are shown in the right panel of fig.4. In this case we find a reasonable correlation especially for the set C, with two exceptional data points which correspond to $^{64}$Ge and $^{78}$Ge. A simple fitting gives the value $q = 0.65$ ($0.59$) including (excluding) these exceptional data. Thus we adopt the value $q = 0.6$ in the following study. This value is much smaller than that adopted in other model spaces consisting of a complete one major shell, indicating the insufficiency of the present model space.

For the evaluation of eq.(2), we utilize the prescription in ref.[21] to take summation over all intermediate states. Here, we need the excitation energies of the intermediate $1^+$ states. Experimentally, the excitation energy of the lowest $1^+$ state is 0.044 MeV (0.075 MeV) in $^{76}$As ($^{82}$Br), while our shell model gives 0.286 MeV (0.470 MeV) for this energy. We can take two options: (1) to use the shell-model excitation energies as they are, and (2) to shift the shell-model energies of all intermediate states commonly so as to reproduce the experimental value of $E_x(1^+)$. The results are summarized in table 2. It can be seen that the shell model adopting the quenching factor $q = 0.6$ reasonably reproduce the experimental values for both $^{76}$Ge and $^{82}$Se. The energy shift of the intermediate $1^+$ states enhances the matrix element by about 8% and 15% for $^{76}$Ge and $^{82}$Se, respectively. The agreement with the experimental value is better in $^{76}$Ge than $^{82}$Se, suggesting the importance of the missing orbits in the present f5pg9-space such as the $g_{7/2}$ orbit for heavier nuclei.

For comparison, other shell-model results [23] are also listed in the same table. In this case, the model space was the same as the present one, but the effective interaction was determined by fitting to 60 energy data of Ni isotopes and $N=50$ isotones based on the G-matrix interaction by Kuo. It can be seen that our interaction gives much smaller nuclear matrix elements than that in ref. [23]. If we just borrow the typical quenching factor $q = 0.74$ from the pf-shell, the results in ref. [23] also reasonably describe the experimental values. Thus it is very important to choose the model space and the quenching factor consistently for a reliable description.
Table 2. Comparison of the nuclear matrix element $M_{GT}^{(2ν)}$ (MeV$^{-1}$) between the experimental data and the shell-model calculations.

|                | $^{68}\text{Ge}$ | $^{82}\text{Se}$ |
|----------------|------------------|------------------|
| Exp. [22]      |                  |                  |
| Shell-model (present) with $q=0.6$, $E_x(1^+_1)$ from shell-model | $0.127^{+0.006}_{-0.004}$ | $0.090^{+0.002}_{-0.010}$ |
| Shell-model (present) with $q=0.6$, $E_x(1^+_2)$ from experimental data | $0.111$ | $0.106$ |
| Shell-model (present) with $q=1$, $E_x(1^+_1)$ from shell-model | $0.120$ | $0.124$ |
| Shell-model (present) with $q=1$, $E_x(1^+_2)$ from experimental data | $0.308$ | $0.295$ |
| Shell-model [23] with $q=1$, $E_x(1^+_1)$ from shell-model | $0.140$ | $0.164$ |
| Shell-model [23] with $q=1$, $E_x(1^+_2)$ from experimental data | $0.180$ | $0.208$ |

4. Summary

In summary, we have developed a shell-model effective interaction for the f5pg9-shell by modifying a realistic G-matrix interaction. This interaction reasonably describes the complicated structure change in Ge isotopes, while insufficiency of the model space appears in some collective observables. We have found that significant quenching ($q \sim 0.6$) is required for the Gamow-Teller operator in the f5pg9-shell in order to reproduce the known low-lying $\beta$-decay data. By introducing such a quenching factor, the two-neutrino double $\beta$-decay matrix elements for $^{76}\text{Ge}$ and $^{82}\text{Se}$ are successfully described.

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