STRUCTURE OF ODD $^{79,81,83}$Se ISOTOPES WITH PROTON AND NEUTRON EXCITATIONS ACROSS $Z = 28$ AND $N = 40$

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The recently measured experimental data of $^{79,81,83}$Se isotopes have been interpreted in terms of shell model calculations. The calculations have been performed in $f_{5/2}p_{9/2}$ space with the recently derived interactions, namely with JUN45 and jj44b. To study the importance of the proton excitations across the $Z = 28$ shell in this region. We have also performed calculation in $fp_{9/2}$ valence space using an $fp$ effective interaction with $^{48}$Ca core and imposing a truncation. Excitation energies, $B(2)$ values, quadrupole moments and magnetic moments are compared with experimental data when available. Present study reveals the importance of proton excitations across the $Z = 28$ shell for predicting quadrupole and magnetic moments.

Keywords: monopole; collectivity.

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1. Introduction

The development of collectivity, island of inversion and single-particle versus collective phenomena in $40 \leq N \leq 50$ region is the topic of current research for the investigation. Experimental evidence of quadrupole collectivity in the neutron rich Fe and Cr with $N \sim 40$ is recently reported by Crawford et al.[1]. In the novel theoretical work of Zuker et al it was mentioned that the enhanced quadrupole collectivity in this region due to presence of $0g_{9/2}$ and its quasi-$SU(3)$ counterpart $1d_{5/2}$ orbital.[2] The interaction for this space recently proposed by Madrid-Strasbourg group.[3-4]

Also the importance of the inclusion of intruder orbitals from $sdg$ shell in the model space for $fp$ shell nuclei is reported in the literature.[5,7,8,9,10] The similarity between island of inversion around $N = 20$ and collectivity around $N = 40$ in Mn isotopes from $^{63}$Mn onwards is recently reported in.[11] The evolution of collectivity in Ge isotopes with $B(E2)$ measurements have been reported in.[12] In this work it is shown that the $N = 40$ shell closure is collapsed in $^{72}$Ge. However, the $N = 50$ shell closure is persistent in Ge isotopes. Using the intermediate-energy Coulomb excitation collectivity at $N = 50$ for the $^{82}$Ge and $^{84}$Se have been established.[13]

The low-energy systematics of odd-A selenium isotopes and the evolution of the $1/2^-, 5/2^-$ and $9/2^+$ levels is shown in Figure 1. It is visible from the figure that in

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Fig. 1. Experimentally observed systematics of low-lying states in odd-A selenium isotopes covering $N = 40$ to $N = 50$ shell gaps.

$^{77,81}$Se isotopes, the ground state is marked by the $1/2^-$. In case of $^{73}$Se the ground state is $9/2^+$ and it start increasing up to $^{77}$Se, and finally it becomes ground state for $^{83}$Se.

In the present paper we consider neutron-rich odd Se isotopes. The shell model calculation in $f_5/2pg_9/2$ space for Se isotopes is reported in the literature using pairing plus quadrupole-quadrupole interactions. The importance of inclusion of proton $f_7/2$ orbital was pointed out by Cheal et al to explain sudden structural changes between $N = 40$ and $N = 50$ for Ga isotopes. In our recent investigation we successfully explained electromagnetic moments of Ga isotopes by including $f_7/2$ orbital in the $f_5/2pg_9/2$ model space.

The paper is organized as follows. In Section 2 gives details of the shell model (SM) calculations. We will discuss in this section the model space and the effective interactions used in the investigation. Section 3 includes results on the spectra of $^{79,81,83}$Se isotopes and configuration mixing in these nuclei. In Section 4, SM calculations on $E2$ transition probabilities, quadrupole moments and magnetic moments are presented. Finally, concluding remarks are given in Section 5.

2. Details of Model Spaces and Interactions

We have performed calculations in two different shell-model spaces. In case of $f_5/2pg_9/2$ space we employed two recently derived effective shell model interactions, JUN45 and jj44b, that have been proposed for the $1p_{3/2}$, $0f_{5/2}$, $1p_{1/2}$ and $0g_{9/2}$ single-particle orbits. The JUN45, developed by Honma et al. is a realistic interaction based on the Bonn-C potential fitting by 400 experimental binding and excitation energy data with mass numbers $A = 63–96$. Brown and Lisetskiy developed jj44b interaction by fitting 600 binding energies and excitation energies.
with \( Z = 28\text{–}30 \) and \( N = 48\text{–}50 \). The single-particle energies for the \( 1p_{3/2} \), \( 0f_{5/2} \), \( 1p_{1/2} \) and \( 0g_{9/2} \) single-particle orbits employed in conjunction with the JUN45 interaction are -9.8280, -8.7087, -7.8388, and -6.2617 MeV respectively. In the case of the jj44b interaction they are -9.6566, -9.2859, -8.2695, and -5.8944 MeV, respectively. The core is \(^{56}\text{Ni} \), i.e. \( N = Z = 28 \), and the calculations are performed in this valence space without truncation. For the JUN45 and jj44b interactions the single-particle energies are based on those of \(^{57}\text{Ni} \). For JUN45 and jj44b interactions there is a rapid decrease in \( f_{5/2} \) proton single-particle energy relative to \( p_{3/2} \) as the neutrons start filling in \( g_{9/2} \) orbit and it become lower than \( p_{3/2} \) for \( N > 48 \) this is shown in Figure 2.

Fig. 2. Effective proton single-particle energies for Cu isotopes for JUN45 and jj44b interactions.

In the \( fp \) \( g_{9/2} \) valence space, we use a \(^{48}\text{Ca} \) core, where eight neutrons are frozen in the \( v f_{7/2} \) orbital. This interaction was reported by Sorlin et al.\(^{19} \). For this model space we allowed up to a total of four particle excitations from the \( f_{7/2} \) orbital to the upper \( fp \) orbitals for protons and from the upper \( fp \) orbitals to the \( g_{9/2} \) orbital for neutrons. The \( fp \) \( pg \) interaction for \( fp \) \( g_{9/2} \) valence space was built using \( fp \) two-body matrix elements (TBME) from\(^{20} \) and \( rg \) TBME \((p_{3/2}, f_{5/2}, p_{1/2} \text{ and } g_{9/2})\)
orbits) from. 21 For the common active orbitals in these subspaces, matrix elements were taken from. 21 The remaining $f_{7/2}g_{9/2}$ TBME are taken from. 22 The single-particle energies are 0.0, 2.0, 4.0, 6.5 and 9.0 MeV for the $0f_{7/2}$, $1p_{3/2}$, $1p_{1/2}$, $0f_{5/2}$, and $0g_{9/2}$ orbits, respectively.

All calculations in the present paper are carried out at DGCTIC-UNAM computational facility KanBalam using the shell model code ANTOINE. 23

3. Spectra

Shell model results for different model spaces presented in Figures 3-5. Yosinaga et al. 14 previously presented shell model results in $f_{5/2}g_{9/2}$ space for pairing plus quadrupole-quadrupole interaction for odd Se isotopes. Present work will add more information by including $f_{7/2}$ orbital in the model space to study importance of proton excitation across the $Z=28$ shell. Recently we have reported results for even Se isotopes in Ref. 24. The comprehensive comparison of shell model results for three interactions used in the calculations are presented with respect to the experimental data.

3.1. $^{79}$Se

The calculated values of the energy levels of $^{79}$Se with the help of JUN45, jj44b and $fpg$ interactions are shown in Figure 3. All the three interactions correctly reproduced the ground state spin and parity. In case of JUN45, the calculated $9/2^+$, $5/2^+$ lower in energy. The jj44b interaction predicted $9/2^+$ about 200 keV higher in energy. The second $1/2^−$ predicted by all interactions are higher in energy while in experiment they are very close to each other. The positive parity levels predicted by jj44b interaction is higher in energy. All the interaction predict correctly the first negative parity as $1/2^−$, but it is lowered by 52 keV in JUN45 and by 29 keV in jj44b. The experimental sequence of $5/2^−$, $3/2^−$, $5/2^−$, $7/2^−$, $3/2^−$ levels correctly reproduced by jj44b interaction. The negative levels predicted by $fpg$ interaction is higher in energy. In contrast to experimentally observed $13/2^−$ doublet, the shell model predicted these levels more than 300 keV separation between each other. For the $7/2^+_3$ level configuration is $\nu(g_{9/2}^{-3})$ with probability $\sim 13\%$ (JUN45) and $\sim 18\%$ (jj44b), respectively. The calculated occupancies for the ground state for neutron $g_{9/2}$ orbital is 6.57 (JUN45) and 6.97 (jj44b). The JUN45 interaction predicts better results for excitation energies in comparison to the jj44b and $fpg$ interactions.
Structure of odd $^{79,81,83}\text{Se}$ isotopes

Fig. 3. Experimental data for $^{79}\text{Se}$ [24] compared with the results of large-scale shell-model calculations using three different effective interactions.
3.2. \textit{\textsuperscript{81}Se}

The comparison of calculated and experimental positive and negative-parity energy levels of $\textit{\textsuperscript{81}Se}$ is given in Figure 4. Only \textit{fpg} interaction is able to correctly reproduce ground state spin and parity. In \textit{jj44b} interaction the first negative-parity level is different from the experimental ones while JUN45 predicted correctly this level. First two energy levels $7/2^+$ and $9/2^+$ for the positive-parity by both the interactions are in sequence with the experimental data but observed experimental difference of 191 keV predicted by JUN45 at 170 keV and with \textit{jj44b} at 220 keV, respectively. For the ground state i.e. $1/2^-$ level configuration is $\nu(p_{1/2}^{-1})$ with probability $\sim 36\%$ (JUN45) and $\sim 30\%$ (\textit{jj44b}), respectively. The calculated occupancies for ground state for neutron $g_{9/2}$ orbital is 8.15 (JUN45) and 8.12 (\textit{jj44b}). For the $7/2^+$ level configuration is $\nu(g_{9/2}^{-3})$ with probability $\sim 35\%$ (JUN45) and $\sim 31\%$ (\textit{jj44b}), respectively. The calculated occupancies for $7/2^+$ for neutron $g_{9/2}$ orbital is 7.20 (JUN45) and 7.22 (\textit{jj44b}). These results demonstrate importance of neutron $g_{9/2}$ orbital for the ground state. The overall results of JUN45 is in good agreement with experimental data.

3.3. \textit{\textsuperscript{83}Se}

For this isotope the experimental data is very sparse. Figure 5 shows the calculated and experimental levels of $\textit{\textsuperscript{83}Se}$ using JUN45, \textit{jj44b} and \textit{fpg} interactions. The JUN45 and \textit{jj44b} correctly reproducing ground state as $9/2^+$, while \textit{fpg} interaction predicting $1/2^-$ as a ground state. The energy level $1/2^+$ is at 1636 keV in JUN45 and at 2485 keV in \textit{jj44b} while in experiment it is at 360 keV. The $f_{5/2}pgg_{9/2}$ space based interactions predicting $11/2^+$ as first excited positive parity level, while there is no experimental result for this level. The configuration for g.s. as $9/2^+$ is $\nu(g_{9/2}^{-1})$ with probability of $\sim 53\%$ (JUN45), $\sim 46\%$ (\textit{jj44b}) and $\sim 50\%$ (\textit{fpg}), respectively. With both model spaces the first $1/2^-$ having configuration $\nu(p_{1/2}^{-1})$, with the maximum probability for this level is $\sim 70\%$ for \textit{fpg} interaction. In comparison of experimental results of low-lying levels and corresponding high values of theoretical results it is clear that neutrons excitation across $N=50$ shell is important. The calculated results are high in energy which reflects that as we approach towards $N=50$, the calculation should include $d_{5/2}$ orbital in the model space. Because $f_{5/2}pgg_{9/2}$ space is not enough.

In the work of Yoshinaga et al.,\textsuperscript{14} for $\textit{\textsuperscript{79}Se}$ the predicted $1/2^-$ level lies higher in energy compared to experimental data, while with \textit{jj44b} it is close to experimental data with a difference of only 29 keV. In case of $\textit{\textsuperscript{83}Se}$, the results predicted by JUN45 is better than previous result.\textsuperscript{14}

The occupancies of proton and neutron orbitals for $\textit{\textsuperscript{79,81,83}Se}$ isotopes, for the ground state and $1/2^-$ state are shown in Table 1. Also in Figure 6, we shown the proton and the neutron occupation numbers of the different orbitals. The proton occupancies for $d_{5/2}$ orbital increase smoothly at the expense of the $p_{3/2}$ as we move
|     | 81Se                          | EXPT. | JUN45 | jJ44b | fpg |
|---|-----------------------------|-------|-------|-------|-----|
| 2986 | 1/2, 3/2, 5/2              |       |       |       |     |
| 2570 | 1/2, 3/2, 5/2              |       |       |       |     |
| 2253 | 3/2                        |       |       |       |     |
| 2150 | 1/2, 3/2                   |       |       |       |     |
| 2030 | 1/2, 3/2                   |       |       |       |     |
| 1809 | 5/2                        |       |       |       |     |
| 1728 | 5/2                        |       |       |       |     |
| 1520 | 5/2                        |       |       |       |     |
| 5490 | 5/2                        |       |       |       |     |
| 5400 | 5/2                        |       |       |       |     |
| 4919 | 5/2                        |       |       |       |     |
| 2944 | 5/2                        |       |       |       |     |
| 1053 | 5/2                        |       |       |       |     |
| 604  | 5/2                        |       |       |       |     |
| 628  | 5/2                        |       |       |       |     |
| 491  | 3/2                        |       |       |       |     |
| 294  | 3/2                        |       |       |       |     |
| 1023 | 3/2                        |       |       |       |     |
| 170  | 3/2                        |       |       |       |     |
| 172  | 3/2                        |       |       |       |     |
| 125  | 3/2                        |       |       |       |     |
| 85   | 3/2                        |       |       |       |     |
| 28   | 3/2                        |       |       |       |     |
| 152  | 3/2                        |       |       |       |     |
| 1/2  | 3/2                        |       |       |       |     |
| 468  | 5/2                        |       |       |       |     |
| 439  | 5/2                        |       |       |       |     |
| 525  | 5/2                        |       |       |       |     |
| 505  | 5/2                        |       |       |       |     |
| 508  | 5/2                        |       |       |       |     |
| 491  | 5/2                        |       |       |       |     |
| 525  | 5/2                        |       |       |       |     |
| 491  | 3/2                        |       |       |       |     |
| 525  | 3/2                        |       |       |       |     |
| 505  | 3/2                        |       |       |       |     |
| 508  | 3/2                        |       |       |       |     |

Fig. 4. The same as in Fig. 2, but for 81Se.
Fig. 5. The same as in Fig. 2, but for $^{83}$Se.
from $^{79}$Se to $^{83}$Se. In case of $f_{pg}$ interaction the occupancies of $f_{7/2}$ orbital is very dominant this reflects importance of inclusion of this orbital in the model space. The neutron occupancies for $g_{9/2}$ orbital increase smoothly at the expense of the $p_{3/2}$ and $f_{5/2}$ orbitals as we move from $^{79}$Se to $^{83}$Se. This reveals the importance of neutron excitation across $N = 40$.

Table 1. Occupation of proton and neutron orbitals for $^{79,81,83}$Se isotopes in $f_{5/2}$ $p_{9/2}$ and $f_{pg}$ $p_{9/2}$ spaces.

| Interaction | Nucleus | $I$ | $\pi 0f_{7/2}$ | $\pi 1p_{3/2}$ | $\pi 0f_{5/2}$ | $\pi 1p_{1/2}$ | $\nu 0p_{3/2}$ | $\nu 0f_{5/2}$ | $\nu 1p_{1/2}$ | $\nu 0g_{9/2}$ |
|-------------|---------|-----|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| JUN45       | $^{79}$Se | $7/2^+_2$ | 2.15 | 3.07 | 0.39 | 0.38 | 3.67 | 5.19 | 1.55 | 6.57 |
|             |         | $1/2^+_1$ | 2.19 | 3.14 | 0.39 | 0.29 | 3.77 | 4.91 | 1.72 | 6.59 |
| jj44b       | $^{79}$Se | $7/2^+_2$ | 2.14 | 3.06 | 0.46 | 0.32 | 3.78 | 4.58 | 1.66 | 6.97 |
|             |         | $1/2^+_1$ | 1.96 | 3.26 | 0.46 | 0.30 | 3.70 | 4.53 | 1.26 | 7.48 |
| fpg         | $^{79}$Se | $7/2^+_2$ | 7.60 | 3.99 | 0.43 | - | 3.59 | 5.30 | 1.14 | 6.07 |
|             |         | $1/2^+_1$ | 7.72 | 3.82 | 0.42 | - | 3.69 | 5.51 | 1.30 | 6.50 |
| JUN45       | $^{81}$Se | $7/2^+_2$ | 2.19 | 3.18 | 0.33 | 0.29 | 3.92 | 5.93 | 1.95 | 7.20 |
|             |         | $1/2^+_1$ | 1.89 | 3.45 | 0.34 | 0.32 | 3.82 | 5.83 | 1.19 | 8.15 |
| jj44b       | $^{81}$Se | $7/2^+_2$ | 2.17 | 3.14 | 0.36 | 0.32 | 3.92 | 5.90 | 1.95 | 7.22 |
|             |         | $1/2^+_1$ | 1.88 | 3.44 | 0.40 | 0.29 | 3.76 | 5.87 | 1.25 | 8.12 |
| fpg         | $^{81}$Se | $7/2^+_2$ | 7.70 | 3.88 | 0.36 | - | 3.95 | 5.95 | 1.96 | 7.14 |
|             |         | $1/2^+_1$ | 7.59 | 4.05 | 0.38 | - | 3.82 | 5.85 | 1.29 | 8.04 |
| JUN45       | $^{83}$Se | $9/2^+_2$ | 2.18 | 3.64 | 0.25 | 0.29 | 3.99 | 5.99 | 1.99 | 9.00 |
|             |         | $1/2^+_1$ | 1.81 | 4.28 | 0.22 | 0.32 | 3.92 | 5.94 | 1.14 | 9.99 |
| jj44b       | $^{83}$Se | $9/2^+_2$ | 2.03 | 3.37 | 0.29 | 0.29 | 3.99 | 5.99 | 1.99 | 9.00 |
|             |         | $1/2^+_1$ | 0.92 | 4.55 | 0.18 | 0.33 | 3.94 | 5.94 | 1.14 | 9.97 |
| fpg         | $^{83}$Se | $9/2^+_2$ | 7.53 | 4.46 | 0.23 | - | 4.00 | 6.00 | 2.00 | 9.00 |
|             |         | $1/2^+_1$ | 7.75 | 5.69 | 0.08 | - | 3.94 | 5.94 | 1.11 | 10.00 |

4. Electromagnetic properties

The calculated $B(E2)$ transition probabilities for both model spaces are given in Table 2. For this effective charges $e_p=1.5$, $e_n=0.5$ are used in the calculation. The

Table 2. $B(E2)$ reduced transition strength in W.u. Effective charges $e_p = 1.5$ $e_n = 0.5$ were used.

|         | $^{79}$Se | $^{81}$Se | $^{83}$Se | $^{79}$Se | $^{81}$Se | $^{83}$Se |
|---------|-----------|-----------|-----------|-----------|-----------|-----------|
| $BE(9/2^+_1 \rightarrow 7/2^+_2)$ |          |          |          |          |          |          |
| Experiment | N/A | 20.37 | 17.65 | 2.40 | JUN45 | 0.05 | 3.20 | 1.37 |
| jj44b     | 27.77 | 17.60 | 0.13 | jj44b | 1.78 | 1.63 | 0.005 |
| fpg       | 32.03 | 10.27 | 9.94 | fpg | 12.13 | 8.09 | 7.84 |
results of quadrupole moments and magnetic moments for the three different interactions are shown in Table 3. The experimental data for quadrupole moments for $^{79}$Se show very good agreement with results of $fpg$ interaction. This shows the importance of inclusion of $\pi f_{7/2}$ orbital in the model space, which was proposed...
Table 3. Electric quadrupole moments, $Q_s$ (in eb), the effective charges $e_p=1.5$, $e_n=0.5$ are used in the calculation and Magnetic moments, $\mu$ (in $\mu_N$), for $g^{eff}_s = 0.7g^{free}_s$.

|          | $^{79}$Se | $^{81}$Se | $^{83}$Se | $^{79}$Se | $^{81}$Se | $^{83}$Se |
|----------|----------|----------|----------|----------|----------|----------|
| $Q(7/2^+)$ |          |          |          |          |          |          |
| Experiment | +0.8 (2) | N/A      | N/A      | Experiment | -1.018 (15) | N/A      | N/A      |
| JUN45     | +0.38    | +0.53    | +0.16    | JUN45     | -1.17     | -1.15    | -1.03    |
| jj44b     | +0.59    | +0.55    | +0.31    | jj44b     | -1.29     | -1.13    | -1.16    |
| fpdg      | +0.65    | +0.60    | -0.07    | fpdg      | -1.20     | -1.24    | +2.47    |
| $Q(9/2^+)$ |          |          |          |          |          |          |
| Experiment | N/A      | N/A      | N/A      | Experiment | N/A      | N/A      | N/A      |
| JUN45     | +0.09    | +0.22    | +0.49    | JUN45     | -1.03     | -1.27    | -1.35    |
| jj44b     | +0.20    | +0.30    | +0.60    | jj44b     | -1.37     | -1.23    | -1.45    |
| fpdg      | +0.25    | +0.49    | +0.61    | fpdg      | -1.09     | -1.43    | -1.35    |
| $Q(5/2^+)$ |          |          |          |          |          |          |
| Experiment | N/A      | N/A      | N/A      | Experiment | N/A      | N/A      | N/A      |
| JUN45     | -0.002   | +0.01    | -0.01    | JUN45     | -0.93     | -1.54    | -1.72    |
| jj44b     | -0.11    | +0.28    | +0.14    | jj44b     | -1.02     | -1.76    | -1.16    |
| fpdg      | -0.03    | +0.32    | +0.12    | fpdg      | -1.15     | -1.63    | +0.65    |

The experimental data for magnetic moments are available only for $^{79}$Se. In Table 3, we compare calculated values of magnetic moments with the experimental data for $^{79}$Se. We also have presented predicted values of magnetic moments by the three interactions for the remained isotopes considered. It is seen from Table 3 that for the $^{79}$Se calculated values of magnetic moments are in better agreement with the experiment when JUN45 interaction is used. From Table we can see that the transition rates are strongly enhanced while the quadrupole moments are of the order of the single-particle ones. The large $B(E2)$ values are due to strong dynamical collectivity as these nuclei of this region lose the magicity properties.

5. Conclusions

We have reported shell model results for neutron-rich odd Se isotopes for two spaces: full $f_{5/2p9/2}$ space and $fp9/2$ space with $^{48}$Ca core. The following broad conclusions can be drawn:

- The energy levels, $B(E2)$’s, quadrupole moments and magnetic moments are in good agreement with the experimental data when available.
• The $E2$ transitions, quadrupole moments and magnetic moments analysis show the importance of proton excitations across $Z = 28$ shell for $f_{pg}9/2$ space.

• Further theoretical development is needed by enlarging model space by including $νd_{5/2}$ orbital to study simultaneously proton and neutron excitations across $Z = 28$ and $N = 50$ shell, respectively.

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