Comparison of shell model results for even–even Se isotopes

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Received 19 April 2013
Accepted for publication 20 August 2013
Published 10 September 2013

Abstract

A comprehensive set of shell model calculations for $^{78–84}$Se isotopes have been performed with recently derived interactions, namely JUN45 and jj44b for $f_5/2p_9/2$ space. To study the importance of the proton excitations across a Z = 28 shell, in this region mentioned by Cheal et al (2010 Phys. Rev. Lett. 104 252502), calculations for $fp_{9/2}$ valence space using an fp effective interaction with $^{48}$Ca as the core, and imposing a truncation, have also been performed. Comparison of the calculations with experimental data show that the predicted results of the jj44b interaction are in good agreement with experimental data.

PACS numbers: 21.60.Cs, 27.50.+e

(Some figures may appear in color only in the online journal)

1. Introduction

The nuclei near the Z = 28 region are the subject of intense research, both experimentally and theoretically [1–3]. In particular, the region of neutron-rich nuclei around $N = 40–50$ shows an evolution of shell structure. The nucleon–nucleon interaction, the spin–orbit, the tensor part and three-body effect play important roles in the shell evolutions. Due to tensor interactions, the nuclear mean field undergoes variations with neutron excess. This leads to monopole migration, which is observed on both sides of the stability line. As we approach the neutron drip line, the neutron density becomes very diffused, which can also leads to shell quenching. Further motivation for nuclear structure studies are to understand other open questions, such as, how does the filling of neutron orbitals beyond $N = 28$ around $^{48}$Ca influence the shell structure? What is the role of the tensor part of proton–neutron interactions? how does the spin–orbit splitting between $f_{5/2}$ and $f_{7/2}$ evolve when approaching $N = 50$? And what is the specific role of particle–hole excitations through Z = 28 and $N = 40$ shell gaps for the onset of deformation below and above $^{78}$Ni?

To study the proton excitations across the Z = 28 gap, many experimental investigations have been performed for Cu [4], Ga [5] and As [6] isotopes. The inversion of $\pi f_{5/2}$ and $\pi p_{3/2}$ orbitals for Cu isotopes have been established, while measuring the magnetic moments for the ground state. In the case of $^{71–81}$Ga isotopes, experimental measurement of spin and moments reveals that there is a structure change between $N = 40$ and 50. The $\pi f_{5/2}$ orbital is dominant in the ground state of $^{79}$Ga and for $^{81}$Ga, the 5/2− level becomes the ground state. The evolution of structure can be seen from the emptying of the $\pi p_{3/2}$ orbital to $\pi f_{5/2}$, which starts as we move from $^{71}$Ga to $^{79}$Ga. Finally $I^\pi = 5/2^−$ becomes the ground state for $^{81}$Ga. In the case of $^{79}$Ga, the $f_{5/2}p_{9/2}$ space fails to correctly explain the magnetic and electric quadrupole moments. Thus, it is crucial to include the $\pi f_{7/2}$ orbital in the model space to study the effect of proton excitations across the Z = 28 effect. In the case of As ($I = 33$), recent experimental investigation by Porquet et al suggests that $f_{5/2}p_{9/2}$ space is not enough to explain the quadrupole excitation built on the 5/2− and 9/2+ state of $^{81}$As [6].

In this work, shell model calculations for $^{78,80,82,84}$Se isotopes in two different model spaces, $f_{5/2}p_{9/2}$ and $fp_{9/2}$, have been performed. The aim of this paper is to study the importance of proton excitations across the Z = 28 gap. One of the authors recently reported the importance of the $\pi f_{7/2}$ orbital for predicting moments of Ga isotopes [7]. In figure 1,
the systematics of $2^+$ for Ni to Se are shown. This figure shows the persistence of $N = 50$ shell closure while $N = 40$ disappears as we move from Ni to Se.

In section 2 details about shell model calculations are given, then spectroscopic results for even–even $^{78,80,82,84}$Se are presented in section 3. In section 4, transition probability, quadrupole moments and occupation numbers are presented. Finally section 5 gives the concluding remarks.

2. Details of model spaces and interactions

The present shell model calculations have been carried out in the $f_{5/2}p_{9/2}$ and $f_{p9/2}$ spaces. In the $f_{5/2}p_{9/2}$ valence space the calculations have been performed with the interactions JUN45 [8] and jj44b [5]. The JUN45 interaction is based on the Bonn-C potential, the single-particle energies and two-body matrix elements (TBMEs) were modified empirically so as to fit 400 experimental data out of 69 nuclei with $A = 63–69$. In the fitting of the JUN45 interaction, the experimental data are taken around $N = 50$. Thus, with this interaction the shell-model results with $N \sim 50$ chain show reasonable agreement with experimental data. The jj44b interaction was obtained from a fit to about 600 binding energies and excitation energies with 30 linear combinations of the good $J–T$ TBMEs. For jj44b, the energy data for the fit were taken from nuclei with $Z = 28–30$ and $N = 48–50$. The rms deviation between experiment and theory for the energies was 250 keV. The single-particle energies for the $p_{1/2}$, $f_{5/2}$, $1p_{1/2}$ 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 $^{56}$Ni, i.e. $N = Z = 28$, and the calculations are performed in this valence space without truncation.

In the $f_{p9/2}$ valence space, we use a $^{48}$Ca core, i.e. only the protons are active in the $f_{1/2}$ orbital, and the interaction $f_{p9/2}$ was reported by Sorlin et al [9]. The $f_{p9/2}$ interaction was built using $f$-p TBME from [10] and rg TBME ($p_{1/2}, f_{5/2}, p_{1/2}$ and $g_{9/2}$ orbits) from [11]. For the common active orbitals in these subspaces, matrix elements were taken from [11]. As the latter interaction (rg) was defined for a $^{56}$Ni core, a scaling factor of $A^{-1/3}$ was applied to take into account the change of radius between the $^{48}$Ca and $^{56}$Ni cores. The remaining $f_{7/2}g_{9/2}$ TBME were taken from [12].

The single-particle energies are 0.0, 2.0, 4.0, 6.5 and 9.0 MeV for the $0f_{7/2}$, $1p_{1/2}$, $1p_{1/2}$, $0f_{7/2}$ and $0g_{9/2}$ orbits, respectively. Since the dimensionality of this valence space is prohibitively large, we have introduced a truncation by allowing $t_r$ particle–hole excitations from the $πf_{7/2}$ orbital to the upper fp orbitals ($p_{1/2}$, $f_{5/2}$, $p_{1/2}$) for protons and $\bar{t}_r$ particle–hole excitations from the upper fp orbitals to the $v_g/2$ orbital for neutrons. The maximum allowed value for $t_r$ and $\bar{t}_r$ is four. The maximal dimension 165 000 813 ($\sim 10^9$) is reached for positive parity in the case of $^{78}$Se when using $f_{3/2}p_{9/2}$ space with a $^{56}$Ni core, since the neutron number is furthest from the closed shell for this nucleus among the Se isotopes considered in this work. In the case of $^{78}$Se, computing time was $\sim 21$ days for both parity. The calculations were performed with the shell-model code ANTOINE [13].

3. Spectra analysis

The results for the three interactions for different model spaces used in the calculations are presented, with respect to the experiment, in figures 2–5. Earlier shell model results in 28–50 model space for pairing plus quadrupole–quadrupole interaction have been reported in the literature by Yoshinaga et al [14]. Furthermore, this work will add information to the earlier work [14], by including the $f_{1/2}$ orbital in the model space to study the proton excitation across the $Z = 28$ shell. The shell model structure of Se isotopes was discussed in [8] using the JUN45 interaction. The results for the three interactions used in the calculations are presented with respect to the experiment.

3.1. $^{78}$Se

Comparison of the calculated values of the energy levels of $^{78}$Se with the experimental data is shown in figure 2. All the three interactions correctly reproduce the experimental sequence of $0^+_1$, $2^+_1$, $4^+_1$, $6^+_1$, $8^+_1$, $10^+_1$ and $12^+_1$ levels at 614, 1503, 2546, 3585, 4625 and 5784 keV, respectively. In case of JUN45, the calculated $2^+_1$, $4^+_1$ and $6^+_1$ levels are 134, 240 and 251 keV higher than the experimental ones, while remainder $8^+_1$, $10^+_1$ and $12^+_1$ are predicted at 117, 323 and 397 keV lower than the experimental levels. The $2^+_1$ level calculated by jj44b is only 60 keV higher as compared to its experimental counterpart. The difference between experimental and calculated energies is increased by increasing the excited energies reaching 433 keV at $12^+_1$. All the levels calculated by $f_{p9/2}$ interaction are much lower than in the experiment. By increasing the spin the difference between the calculated and experimental levels is increased and it become 1751 keV when reaching the $12^+_1$ level.

In all the calculations, the first two $0^+$ and $2^+$ levels of the second positive-parity band are interchanged with respect to the experimental ones. The next $0^+$ and $3^+$ levels are located higher than in the experiment in all calculations. The experimental sequence levels $2^+$, $4^+$, $4^+$ and $5^+$ at 1996, 2191, 2682 and 2735 keV are better reproduced by the JUN45

![Figure 1. Systematic of the experimentally observed $E(2^+_1)$ for $Z = 28–34$ near the $N = 28$, 40 and 50 shell closure.](image-url)
Table 1. Comparison of experimental and calculated excitation energies of $^{78}$Se with three different interactions.

| Energy (MeV) | EXPT. | JUN45 | jj44b | fpg |
|--------------|-------|-------|-------|-----|
| 0.70         | 614   | 748   | 674   |     |
| 0.73         | 2102  | 1593  | 1683  | 1945 |
| 1.00         | 1654  | 1743  | 1553  | 1628 |
| 1.01         | 1291  | 1150  | 1484  | 1163 |
| 1.06         | 1996  | 2078  | 2078  | 2265 |
| 1.10         | 2121  | 2100  | 2078  | 2265 |
| 1.20         | 2289  | 2336  | 2336  | 2309 |
| 1.25         | 2539  | 2564  | 2564  | 2624 |
| 1.30         | 2647  | 2675  | 2675  | 2778 |
| 1.40         | 2797  | 2855  | 2855  | 2855 |
| 1.50         | 3197  | 3403  | 3403  | 3699 |
| 1.60         | 3107  | 3034  | 3034  | 3069 |
| 1.70         | 3107  | 3034  | 3034  | 3069 |
| 1.80         | 3107  | 3034  | 3034  | 3069 |
| 1.90         | 3107  | 3034  | 3034  | 3069 |
| 2.00         | 3107  | 3034  | 3034  | 3069 |
| 2.10         | 3107  | 3034  | 3034  | 3069 |
| 2.20         | 3107  | 3034  | 3034  | 3069 |
| 2.30         | 3107  | 3034  | 3034  | 3069 |
| 2.40         | 3107  | 3034  | 3034  | 3069 |

Figure 2. Comparison of experimental and calculated excitation spectra of $^{78}$Se with three different interactions.
Figure 3. Comparison of experimental and calculated excitation spectra of $^{80}$Se with three different interactions.
| Energy (MeV) | 82Se | 88Se | 90Se |
|-------------|------|------|------|
| 0+          |      |      |      |
| 2+          |      |      |      |
| 4+          |      |      |      |
| 6+          |      |      |      |
| 8+          |      |      |      |
| 10+         |      |      |      |
| 12+         |      |      |      |
| 14+         |      |      |      |
| 16+         |      |      |      |
| 18+         |      |      |      |
| 20+         |      |      |      |

*Figure 4.* Comparison of experimental [15] and calculated excitation spectra of $^{82}$Se with three different interactions.
Figure 5. Comparison of experimental [16–18] and calculated excitation spectra of $^{84}$Se with three different interactions.
calculation. The two $6^+$ levels appear in all calculations after the $5^+$ level, which has not been observed in the experiment. The last three levels of this band, calculated by the JUN45 interaction, are in excellent agreement with the experimental data. Experimental levels of this band measured up to $10^+$ and many odd spin levels $1^+, 7^+, 9^+$, which appear in the calculations, have not been observed in the experiment. With both the interactions, the most dominant configuration for g.s. is $\pi(p_1^2f_2^2) \otimes \nu(p_1^2f_2^2p_2^2_{1/2}g_9^\pm_{3/2})$. The probability is less than 10% in all wave functions.

The experimental negative-parity levels start with the $3^-$ level. The first negative-parity level is $4^-$ in both JUN45 and jj44b calculations, while it is $2^-$ in the fpg calculation. In the JUN45 calculation the first few levels are more compressed than in the experiment. The spins and parities of $(7^-)$, $(8^-)$, $(9^-)$ and $(9^+)$ levels, which are not confirmed in the experiment, are predicted by all calculations as negative-parity levels. The sequence of experimentally observed levels starting from $1^-$ is exactly the same as in the jj44b calculation. The structure of $3^-$ is $\nu(p_1^2g_9^-)$ with 13% for jj44b.

### 3.2. $^{78}$Se

In figure 3 we have shown the comparison of the values of the energy levels calculated by JUN45, jj44b and fpg interactions with experimental data. The values calculated by JUN45 are in very good agreement with all the levels of the first experimental positive-parity band, which are available up to $10^+$. The jj44b calculation predicts higher values after $4^+$, while the values predicted by the fpg calculation are lower by $4^+$ and then the $6^+$ level is higher. The $8^+$ and $10^+$ levels are again lower than in the experiment.

The first two levels of the second positive-parity band are interchanged with respect to those of $^{78}$Se in the jj44b calculation. The sequence of these levels are not changed with respect to those of $^{78}$Se in the JUN45 calculation. In the fpg calculation, the $2^+$ level is lowest in the second positive-parity band. The $4^+$ levels are predicted much lower than in the experiment, while the second $0^+$ and $2^+$ levels are higher in this band than in the experiment. The second $4^+$ level is only 17 keV higher than in the experiment. Then three $6^+$ levels in succession come in the calculation. The $8^+$ in the calculation is much higher than in the experiment. For odd spin-positive-parities, which we have shown in the third column, all the calculations predict two levels for each spin ($1^+$ and $1^+$, $3^+$ and $3^+$, ...). In the experiment only one $1^+$ and $3^+$ are measured, first of which is higher than all $1^+$ levels in the calculations, while the second of them is lower than the $3^+$ level in all calculations. For $^{80}$Se with both interaction probabilities ~15% but JUN45 have structures $\pi(p_1^2f_2^2) \otimes \nu(p_1^2f_2^2p_2^2_{1/2}g_9^+_{3/2})$ and jj44b have $\pi(p_1^2f_2^2) \otimes \nu(p_1^2f_2^2p_2^2_{1/2}g_9^\pm_{3/2})$.

### Table 1. $B(E2)$ reduced transition strength in W.u. Effective charges $e_p = 1.5, e_n = 0.5$ were used. Experimental values were taken from the NNDC database.

|         | $^{78}$Se | $^{80}$Se | $^{82}$Se | $^{84}$Se |
|---------|-----------|-----------|-----------|-----------|
| BE($2^+_1 \rightarrow 0^+_1$) |
| Experiment | 32.8 (4.5) | 24.2 (0.4) | 16.7 (0.3) | N/A |
| JUN45 | 18.83 | 16.53 | 13.88 | 6.64 |
| jj44b | 20.74 | 18.88 | 15.33 | 8.37 |
| fpg | 30.87 | 24.08 | 16.33 | 8.22 |
| BE($4^+_1 \rightarrow 2^+_1$) |
| Experiment | 38.2 (5.6) | 34.7 (1.1) | 18.7 (3.0) | N/A |
| JUN45 | 25.47 | 21.40 | 19.60 | 1.96 |
| jj44b | 27.23 | 25.65 | 20.77 | 0.005 |
| fpg | 46.27 | 32.85 | 25.86 | 1.42 |
| BE($6^+_1 \rightarrow 4^+_1$) |
| Experiment | 48 (14) | N/A | N/A | N/A |
| JUN45 | 23.69 | 16.81 | 15.42 | 1.02 |
| jj44b | 24.22 | 21.92 | 18.01 | 3.25 |
| fpg | 48.92 | 32.01 | 24.42 | 0.12 |
| BE($8^+_1 \rightarrow 6^+_1$) |
| Experiment | 57 (19) | N/A | 0.56 (0.03) | N/A |
| JUN45 | 13.01 | 7.45 | 0.38 | 0.0008 |
| jj44b | 21.86 | 1.27 | 0.31 | 0.002 |
| fpg | 49.01 | 7.13 | 0.57 | 1.13 |

### Table 2. Electric quadrupole moments, $Q_e$ (in eb), with the three different interactions (the effective charges $e_p = 1.5, e_n = 0.5$ are used in the calculation).

| $Q_e$ (in eb) |
|--------------|
| $^{78}$Se | $^{80}$Se | $^{82}$Se | $^{84}$Se |
| Experiment | | | | |
| JUN45 | $-0.20$ (7) | $-0.31$ (7) | $-0.22$ (7) | N/A |
| jj44b | $-0.13$ | $-0.31$ | $-0.33$ | $+0.01$ |
| fpg | $-0.32$ | $-0.36$ | $-0.37$ | $-0.27$ |
| | $+0.47$ | $-0.35$ | $-0.36$ | $+0.04$ |
| Experiment | $+0.17$ (9) | N/A | N/A | N/A |
| JUN45 | $+0.13$ | $+0.28$ | $+0.24$ | $-0.09$ |
| jj44b | $+0.30$ | $+0.35$ | $+0.27$ | $+0.13$ |
| fpg | $-0.33$ | $+0.36$ | $+0.28$ | $+0.007$ |
| Experiment | $-0.68$ (15) | N/A | N/A | N/A |
| JUN45 | $-0.09$ | $-0.35$ | $-0.39$ | $+0.10$ |
| jj44b | $-0.36$ | $-0.40$ | $-0.42$ | $+0.18$ |
| fpg | $+0.63$ | $-0.29$ | $-0.43$ | $+0.15$ |

### 3.3. $^{82}$Se

As is seen from figure 4, all calculated levels in the first column are in a similar pattern to the experimental one. Better values are predicted by the JUN45 calculation.

In all calculations the first level in the second column is the $0^+$ level, like in the experiment. The closest value of this level is predicted by JUN45. The spacing between the first and the second $2^+$ levels in the second column are less than that in the experiment in all calculations. In the JUN45 calculation, the first of the two $4^+$ levels is located lower, while the second one is higher, than in the experiment. In the jj44b calculation, both of them are much higher than in the experiment. In the fpg calculation, the first $4^+$ is only 8 keV higher than in the experiment. The second $0^+$ is predicted well by the jj44b calculation. For $^{82}$Se, both JUN45 and jj44b
are predicted better the agreement of the all calculated values of negative-parity levels with the experimental data is very much improved compared to the calculations. Also the 6+ level is a little bit higher than in JUN45, where spacings between the levels are very like experimental ones.

In all calculations, the first positive-parity level in the second column is 0+ as in the experiment. The sequences of 01+, 02+ and 21+, 22+ levels is the same with the experimental one in the jj44b calculation and spacings between them are larger than in the experiment. The sequence of the pair of these levels is different from the experimental one in the JUN45 and fpg calculations and the spacing between them is much larger than in the experiment. The 41+, 42+ and 43+ levels are located much lower than in the experiment in all calculations. For the ground state, all the orbitals are completely filled like experimental ones.

As is seen from figure 4 agreement of the all calculated values of negative-parity levels with the experimental data is very much improved compared to the 78,80Se isotopes.

3.4. 84Se

The levels of the first column of figure 5 are predicted better by the jj44b calculation. Also the 6+ level is a little bit higher than in JUN45, where spacings between the levels are very experimental ones.

In all calculations, the first positive-parity level in the second column is 0+ as in the experiment. The sequences of 01+, 02+ and 21+, 22+ levels is the same with the experimental one in the jj44b calculation and spacings between them are larger than in the experiment. The sequence of the pair of these levels is different from the experimental one in the JUN45 and fpg calculations and the spacing between them is much larger than in the experiment. The 41+, 42+ and 43+ levels are located much lower than in the experiment in all calculations. For the ground state, all the orbitals are completely filled with maximum probability of 40%. The structure of 01+ is $\pi (f_{5/2}^4) \otimes \nu (p_{3/2}^4 f_{5/2}^4 p_{1/2}^2 g_{9/2}^2)$ with probability 33% (JUN45) and 57% (jj44b).

The 1+ and 3+ levels that appear in the calculations have not been measured in the experiment. The measured 5+ level...
is predicted better by JUN45. The $7^+$ level is located very high in all the calculations as compared to the experimental one.

The structure of the negative-parity levels for $^{84}$Se changed drastically compared to previous isotopes, and both of the JUN45 and jj44b calculations fail to explain it.

For $^{78}$Se in [14], the predicted $0^+_2$ state lies lower in energy compared to experimental data, while in the present work with the jj44b interaction the result is close to experimental data with a difference of only 95 keV. In the case of $^{82}$Se, the predicted energy gap between the $6^+_1$ and $8^+_1$ states is correctly reproduced, while in [14] these levels are very close to each other.

4. Transition probability, quadrupole moments and occupation numbers analysis

4.1. E2 transition probability and quadrupole moments

The calculated $B(E2)$ transitions are shown in table 1. In the case of $^{78,80}$Se, the results predicted by the fpg interaction show better agreement with experimental data. While for $^{82,84}$Se, the jj44b interaction results are more reasonable. Thus, we may conclude that proton excitation across the $Z = 28$ shell for lighter Se isotopes are important. In the present study our predicted results for $B(E2)$ values are close to experimental data, in comparison with [14]. The results of the $B(E2)$ transitions for the fpg interaction are probably related to the contribution of the protons in the $f_{7/2}$ orbital, which could be compensated for with smaller effective charges. However with JUN45 and jj44b, due to a missing proton $f_{7/2}$ orbital, we need a higher value of effective charges. To see the effect of the inclusion of a proton $f_{7/2}$ orbital in the model space, we keep the effective charges the same.

We have also calculated static quadrupole moments, as shown in table 2. For the first $2^+$ state, the JUN45 and jj44b interaction correctly predicts the sign of quadrupole moments for $^{78,80,82}$Se. The fpg interaction predicts a positive sign for $^{78}$Se. The overall agreement for quadrupole moments predicted by jj44b is better.

4.2. Occupation numbers

In figure 6, we show the proton/neutron occupation numbers of fpg-shell orbits for $0^+_1$ and $2^+_1$ levels. The proton occupancies increase smoothly in the $f_{5/2}$ orbital, while $p_{3/2}$ is decreasing. But beyond $N = 46$, in the case of the JUN45 interaction, the change in occupancy of these two orbitals is very significant. With both interactions the occupancy of proton $p_{1/2}$ and $g_{9/2}$ orbitals are similar. As the neutron number increases, the occupation number of the $v g_{9/2}$ orbital increases drastically. The neutron number occupation shows a similar distribution for $2^+_1$ as in the ground state.

5. Summary

In summary, a comprehensive study for the structure of neutron-rich even–even Se isotopes has been carried out using large-scale shell-model calculations for two spaces: full $f_{5/2}g_{9/2}$ space and $f_{7/2}g_{9/2}$ space with $^{48}$Ca core. The following broad conclusions can be drawn:

- The overall calculated results for the energy levels, $B(E2)$s and quadrupole moments are in good agreement with the experimental data.
- The $E2$ transitions, quadrupole moments analysis shows the importance of proton excitations across the $Z = 28$ shell for $f_{9/2}$ space.
- For $^{78–80}$Se, the $B(E2)$ values predicted by fpg transitions are in better agreement with experimental data.
- The result (wave functions) of $^{82}$Se may be used for calculating nuclear transition matrix elements and finally the half-live for this nucleus, which is a good candidate for neutrinoless double beta decay.
- It is also important, while tuning the effective interaction, that we can also take experimentally known quadrupole moment as a parameter to increase the predictive power of effective interaction.
- Further, theoretical development is needed by enlarging model space by including the $v d_{5/2}$ orbital to simultaneously study proton and neutron excitations across the $Z = 28$ and 50 shells, respectively.

Acknowledgments

Thanks are due to E Padilla–Rodal for useful discussions during this work. All the shell-model calculations have been performed at the KanBalam computational facility of DGCTIC-UNAM, Mexico. MJE acknowledges support from grant no. 17901 of CONACyT projects CB2010/155633 and F2-FA-F177 of Uzbekistan Academy of Sciences.

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