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Shell Model Description of N = 51 Isotones

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Abstract: *Shell model calculations for ^{83}Ge, ^{85}Se, ^{87}Kr, ^{89}Sr and ^{91}Zr nuclei which form the N = 51 isotonic chain have been reported. The calculations have been performed taking ^{78}Ni as a core and the valence space comprises of $\nu(0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2})$ orbitals for neutrons and $\pi(0f_{5/2}, 1p_{3/2}, 1p_{1/2}, 0g_{9/2})$ orbitals for proton. The effective interaction for the present calculations is based on CD-Bonn N − N potential and adopted to the model space based on the ^{78}Ni core. The results of present calculations show that the chosen interaction does not give a good agreement of the observed spectra with the experimental data for N=51 isotones. However some general trends of the experimental spectra like increase in the $E(1/2^+)$~ $E(5/2^+)$ energy splitting and raising of $3/2^+$ level in going from Z=32 to 40 are well reproduced.*
Keywords- *Isotones; effective interaction*

I. Introduction

With the development of first generation radioactive ion beam facilities over the last decade it is now possible to access very neutron rich nuclei in few specific regions of the nuclear chart which do not even survive on the earth. Further, the study of these nuclei is considered as an ideal testing ground for a number of important issues: e.g. the evolution of shell structure concentrating on the neutron rich regions around Z = 20 and 28, relation between single particle and collective behavior etc. The study of nuclei with two magic numbers Z = 28 and N = 50 and in its vicinity has already been undertaken for a long time towards and beyond ^{78}Ni and is still the objective of active experimental and theoretical research. Previously neutron rich nuclei in the vicinity of ^{78}Ni have been produced and studied using deuteron beam available at the Tandem Accelerator in Orsay[1]. Since 78Ni is the most neutron rich example of doubly magic nucleus in whole nuclide chart with an extreme N/Z ratio of 1.79 and further away from the stability on the neutron rich side, this region of nuclide chart remains extremely hard to reach experimentally. So far, only a dozen of ^{78}Ni could be successfully synthesized and identified with most advanced techniques of production of rare isotopes using high energy beam fragmentation. The most practical method of exploring the ^{78}Ni region is to study the decay of fission product to the levels of the N = 50 isotones above ^{78}Ni [2] and the study of nuclei with few valence particle or holes provides best testing ground for the basic ingredients of the shell model calculations. So N = 51 nuclide form an interesting example of nuclei where the variation of the neutron single-particle energies can be investigated and nuclei in this mass region are particularly important to understand astrophysical processes. Also neutron rich nuclei between N = 50 and N = 82 shells cover waiting point in r-processes. Properties of low lying states in these nuclei near closed shell are useful for the description of nuclear structure, quenching of shell gaps and a more uniform spacing of single-particle energy levels [3,4,5] and influence how heavier nuclei are produced in astrophysical rapid neutron capture (r−) process [6,7]. A large number of nuclei can be populated by means of binary reactions such as multinucleon transfer and deep inelastic collisions with a stable beam. Such reactions combined with modern -detection array have increased substantially the available data on nuclei far from stability. Recently an experiment has been performed at LNL to study the nature of the low lying yrast or quasi yrast $7/2^+$ states in 32 < Z < 40, N = 51 nuclei in order to assess their collective or $\nu 1g_{7/2}$ single-particle origin and better constrain the relative position of the latter with respect to other neutron single-particle states above a ^{78}Ni core [8].

In the present work we have chosen N = 51 isotone nuclide viz. ^{83}Ge, ^{85}Se, ^{87}Kr, ^{89}Sr and ^{91}Zr which form an interesting region to study the validity of nuclear shell model in modeling of the available nuclear data [9,10]. Recently single neutron transfer reaction have been measured on two N= 50 isotones at HRIBF. The single particle like states of ^{83}Ge and ^{85}Se have been populated using radioactive ion beams of ^{82}Ge and ^{84}Se and the (d, p) reaction in inverse kinematics. This experiment has provided data on level structure of ^{83}Ge and ^{85}Se [9] including data on ^{87}Kr, ^{89}Sr and ^{91}Zr with references therein.

The nuclear shell model is the most powerful tool for giving a quantitative interpretation to the experimental data. Our recent shell-model (SM) studies for neutron-rich F isotopes [11], odd and even isotopes of Fe [12,13], odd-odd Mn isotopes [14] odd-mass ^{61,63,65}Co isotopes [15], even-even Ni and Zn and odd-A Cu isotopes [16,17], odd-mass Ga isotopes [18] and neutron deficient $^{102-108}$Sn isotopes [19] have shown that the shell model calculations, carried out in an extended configuration space with suitably renormalized effective interaction, give a satisfactory account of the experimental data of unstable nuclei. Following this in the present work we have performed large scale shell model calculation for neutron rich ^{83}Ge, ^{85}Se, ^{87}Kr, ^{89}Sr and ^{91}Zr nuclei which form the N = 51 isotonic chain. The effective interaction used in the present work is renormalized G matrix obtained from CD Bonn N-N interaction and adopted to the model space based on a ^{78}Ni core (referred to as jj45pna interaction). Earlier jj45pna interaction has been used in the study of ^{128}Cd [20] and its monopole corrected version in the study of Zr isotopes in this region [21]. G-matrix derived from CD-Bonn potential have also been widely used in the theoretical calculations performed by the Oslo group and their coworkers in ^{132}Sn region [22,23,24,25,26].

The aim of this work is to test the suitability of the model space and the effective interaction in interpreting the experimental data of these highly unstable nuclei on the neutron rich side. The paper is organized as follows: section 2 gives details of the calculation. Results and discussion are given in section 3. Finally in section 4 conclusions are given.

II. Details of Calculation

2.1. Configuration Space

Large scale shell model calculations have been performed for even Z neutron-rich N = 51 isotones in mass region A=83 - 91 treating ^{78}Ni as a core. The configuration space comprises of $\nu(0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, $0h_{11/2})$ orbitals for neutrons and $\pi(0f_{5/2}$, $1p_{3/2}$, $1p_{1/2}$, $0g_{9/2})$ orbitals for protons with all Pauli allowed combinations of valence particles. The calculated single particle energies for model space $\pi(0f_{5/2}$, $1p_{3/2}$, $1p_{1/2}$, $0g_{9/2})$ and $\nu(0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, $0h_{11/2})$ are respectively -0.7166, 1.1184, 1.1262 and 0.1785 MeV for proton orbitals and 5.7402, 2.4422, 2.5148, 2.1738 and 2.6795 MeV for neutron orbitals.

2.2. Effective Interaction

The calculations have been performed with a state of art effective interaction (jj45pna) derived from high precision, charge dependent version of Bonn N-N potential, known as CD-Bonn potential, see ref.[27]. The parameter of the potential fit the proton- proton and neutron-proton data available till 2000 with χ^2 per datum close to 1. This high precision is obtained by the introduction of the two effective σ mesons the parameters of which are partial wave dependent. The charge dependence of the CD-Bonn potential is based upon the predictions by the Bonn full model[28] for charge symmetry and charge independence breaking in all partial wave with $J \leq 4$. The strong short range repulsion is overcome by Brueckner (reaction) G-matrix renormalization which accounts for the effects of two nucleon correlations [29]. The jj45pna effective interaction has been obtained by adopting G-matrix to the chosen model space above the ^{78}Ni core by using many body perturbation technique.

2.3. Computer Code

The calculations have been performed with the code NuShell [30]. It comes with a library of model spaces and interactions. This shell model code has been developed by Alex Brown from MSU to tackle the dimensions up to 10^6 in the J − T scheme and about $2x10^7$ in m-scheme. NuShell generates the basis states in m-scheme and then computes the matrix in j-scheme. Therefore, it bypasses the complication of angular momentum algebra in j − j coupled basis and also avoids the huge matrix dimension generated during m-scheme. NuShell consists of seven main programs and some supporting codes.

III. Results and Discussion

3.1. Excitation Energies

The results of our calculations for different isotones are shown in Figs 1-5 along with the experimental data for comparison . The excited states up to 2.5 MeV have been calculated. Experimentally it is well established that the $\nu 1d_{5/2}$ subshell is the ground state for all the isotones considered here i.e. $1d_{5/2}$ is first valence orbit above the N=50 shell gap which is well reproduced in our results for all isotones. Our calculations predict $1/2^+$ as the first excited state in agreement with the experimental data for all the isotones considered, except for ^{91}Zr in which $7/2^+$ state is predicted as the first excited state and $1/2^+$ state lies slightly higher. The predicted $E(1/2^+)$ state lies lower than the corresponding experimental values in all the cases. The special feature of the experimental energy spectra of N = 51 isotones is increase in the $E(1/2^+)$-$E(5/2^+)$ splitting in going from Z= 32 to Z=40. This trend is also reproduced in the theoretical spectra.

The variation of the excitation energy of first $1/2^+$ state with proton number is shown in Fig 6. If energies relative to the $2s_{1/2}$ are considered, the monopole residual interaction between spin-flip $\Delta\ell=1$ pair of $0f_{5/2}$ proton orbital and $1d_{5/2}$ neutron orbital could be lowering $1d_{5/2}$ excitation with respect to $2s_{1/2}$ orbital as the stable ^{89}Sr and ^{91}Zr are approached. Since $1/2^+$ level is attributed to the excitation of neutron to $2s_{1/2}$ level, this variation of $E(1/2^+)$ with filling of proton orbitals is a signature of monopole effect [9,10]. Alternatively the raising of the $2s_{1/2}$ orbital in neutron rich N=51 isotones could be evidence for a reduced diffuseness of the nuclear suface, which preferentially raises $2s_{1/2}$ orbitals relative to the increased binding of lower j-states [31].

In all the isotones with the exception of ^{91}Zr, the $7/2^+$ level is predicted to lie higher than the $3/2^+$ level contrary to the experimental results. $7/2^+$ state for ^{85}Se and ^{87}Kr have small deviations from corresponding experimental values. For ^{83}Ge its value is too high and for ^{89}Sr and ^{91}Zr its value is too low in comparison to the experimental data. So this interaction gives poor results for $7/2^+$ state. It finally becomes first excited state for ^{91}Zr. This indicates that the considered model space is not enough for ^{91}Zr.. Rising trend of calculated $E(3/2^+)$ values with increasing Z is supported by the experimental data although their values are comparatively low. $7/2^+$ state is single particle energy in nature with weaker amount of mixing of neutron single particle $0g_{7/2}$ with coupled configuration. On the other hand $3/2^+$ state is single particle energy in nature with partial mixing of neutron single particle $1d_{3/2}$ with coupled configuration [32]. Single particle energies used in our calculations are 5.7402 for $0g_{7/2}$ and 2.5148 for $1d_{3/2}$. The calculated levels are sensitive to the single particle energies of the neutron orbitals which in turn get renormalized due to the monopole correction. Thus use of effective single particle energies can change the results.

The agreement of the $E(9/2^+)$ with experimental data for ^{89}Sr and ^{91}Zr is reasonably good. For ^{87}Kr and ^{85}Se Theoretical $E(9/2^+)$ levels lie higher as compared to the corresponding experimental values but rising trend of $E(9/2^+)$ state with increasing Z shows the nearly correct systematic for all nuclei. The experimental data for $E(9/2^+)$ state for ^{83}Ge is not available and theoretically predicted value is 1.856 MeV. The $9/2^+$ state is likely to have a rather pure coupled configuration $\nu 1d_{5/2} \otimes 2^+$, as $0g_{9/2}$ orbit is too deeply bound (by about 3.5 MeV) to give a fraction of single particle state at low energy . Such a configuration for the $9/2^+$ state is confirmed by the fact that its energy follows closely that of the 2^+ state [33].

The discrepancy between the calculated values and the experimental data can also be attributed to the core excitation effect and neglect of contributions arising due to 3N forces [34] . The coupling of the $\nu 1d_{5/2}$ orbit to the first 2^+ excitation of the core provides a multiplet of states with spin between $1/2^+$ and $9/2^+$. Therefore the $1/2^+$, $3/2^+$ and $7/2^+$ states originating from the $2s_{1/2}$,$1d_{3/2}$ and $0g_{7/2}$ orbits can be mixed to those obtained with the coupling to the core excitation. But experimentally $1/2^+$ and $7/2^+$ significantly depart from that of 2^+ core indicating that their composition is likely to be mostly of single particle origin with a weaker amount of mixing with the coupled configuration. So they are originating mainly from $2s_{1/2}$ and $0g_{7/2}$ subshell [33] and observed as first and second excited state experimentally. While $3/2^+$ state close to one of 2^+ state of core [10] is originating with a partial mixing of neutron single particle state $1d_{3/2}$ with coupled configuration [32]. Recent studies [35-37] have shown that 3N forces play an important role in the evolution of shell structure in neutron rich nuclei. Explicit calculations carried out for neutron rich light mass oxygen [35] and medium mass calcium isotopes [36] have shown that 3N forces add a repulsive term to the monopole component of the two nucleon interaction and are key to explain the doubly magic nature of ^{24}O and ^{48}Ca nuclei. Inclusion of 3N forces substantially increases the energy gap between $0d_{5/2}$ and $1s_{1/2}$ levels in oxygen and between $0f_{7/2}$ and $1p_{3/2}$ levels in calcium leading to shell closure at N=16 and N=28. Three body forces also play an important role in the nuclear saturation properties in nuclear matter [37] ,which can be demonstrated typically in the Bruckener (G-Matrix) theory. Thus 3N forces are likely to play an important role in the ^{78}Ni region as well. The poor agreement of the$1/2^+$ single particle states with the experimental levels is an indication of the importance of 3N component in the interaction. Such forces, if included ,will shift the levels upwards due to increased repulsion and are likely to improve the agreement with the experimental data.

3.2. Wave Function

Most dominant configuration of wave function for ground state and first three excited states for all the isotones are shown in table II. It is observed that in all the isotones except in ^{91}Zr, the structure of the proton part of the wave function for the ground state and first excited state $1/2^+$ remains the same confirming that the excited state is due to the excitation of neutron from $(d_{5/2})$ to $(s_{1/2})$. In ^{91}Zr the structure of the proton wave function changes indicating the more complex nature of $7/2^+$ and $1/2^+$ excitations. In ^{83}Ge and ^{87}Kr the proton wave functions for $7/2^+$ state remains unchanged whereas in ^{85}Se, ^{89}Sr and ^{91}Zr their structure changes. The proton wave function for $3/2^+$ state also remains same in all the isotones except for ^{91}Zr. The difference can be attributed to the variation in proton single particle energies with changing Z.

3.3. Electromagnetic Properties

Theoretically calculated B(E2) values for the transition $1/2^+ \rightarrow 5/2^+$ and $7/2^+ \rightarrow 5/2^+$ are shown in table III for each of the N=51 isotonic nuclei. The effective charges used for proton and neutron are e_π^{eff} = 1.50 and e_ν^{eff} = 0.5 respectively. The calculations show that $B(E2;\ 1/2^+ \rightarrow 5/2^+)$ values first increase up to ^{87}Kr and then decreases for ^{89}Sr. No experimental data is available for comparison. The decrease in $B(E2;7/2^+ \rightarrow 5/2^+)$ values in going from midshell to ^{89}Sr supports the onset of shell closure at Z=40.

IV. Conclusions

In the present work large scale shell model calculations have been performed for N = 51 isotones nuclide ^{83}Ge, ^{85}Se, ^{87}Kr, ^{89}Sr and ^{91}Zr in valence space $\nu(0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2})$ orbitals for neutrons and $\pi(0f_{5/2}, 1p_{3/2}, 1p_{1/2}, 0g_{9/2})$ orbitals for protons with ^{78}Ni core. The effective interaction is based on the renormalization of CD-Bonn nucleon-nucleon potential developed by G - matrix theory for nuclei above ^{78}Ni core. Thus simple and pure neutron configurations of $(1d_{5/2})^{1\nu}$ and $(2s_{1/2})^{1\nu}$ above the N=50 shell closure can be assumed to describe the ground state and first excited state of all isotones. Ground state spin $5/2^+$ for all the isotones is associated with the last odd neutron in $d_{5/2}$ state. Similarly $1/2^+$ spin of first excited state can be attributed to the excitation of the last neutron from $1d_{5/2}$ to $2s_{1/2}$ level. The increase in $E(1/2^+)$-$E(5/2^+)$ splitting in going from Z=32 to 40 is direct reflection of the monopole effect wherein the energy of $1/2^+$ state is gradually increasing with the filling of proton orbitals.

The calculated $1/2^+$ levels are consistently lower than the corresponding experimental values. The fitting of higher $3/2^+$,$7/2^+$ and $9/2^+$ states with the corresponding experimental data is not good. Thus, the present interaction in the chosen model space does not give good agreement with the experimental data. The reason for this could be manifold.. Firstly, all these states have admixtures of coupling of single particle states with core excitation. Secondly, it is well known that the neutron single particle orbital changes with filling of proton number due to the attracting monopole pairing interaction between proton and neutron in spin-orbit partners [38]. So minor adjustment in the monopole part of the neutron proton interaction and renormalization of the single particle energies of the neutron orbitals can lead to better agreement with the experimental data. Thirdly, recent studies have shown that 3N forces have important effect on the evolution of shell structure in neutron rich nuclei. The three body component of these interactions gives rise to a repulsive contribution to the monopole interaction. These forces when included can give a shift to $1/2^+$ states in the right direction . Lastly, the wave functions of the $7/2^+$ states in Se, Kr, and Zr and $1/2^+$ and $3/2^+$ states of Zr have main components in which proton configuration is different than the ground state configuration showing that these states are not pure neutron excitation states.

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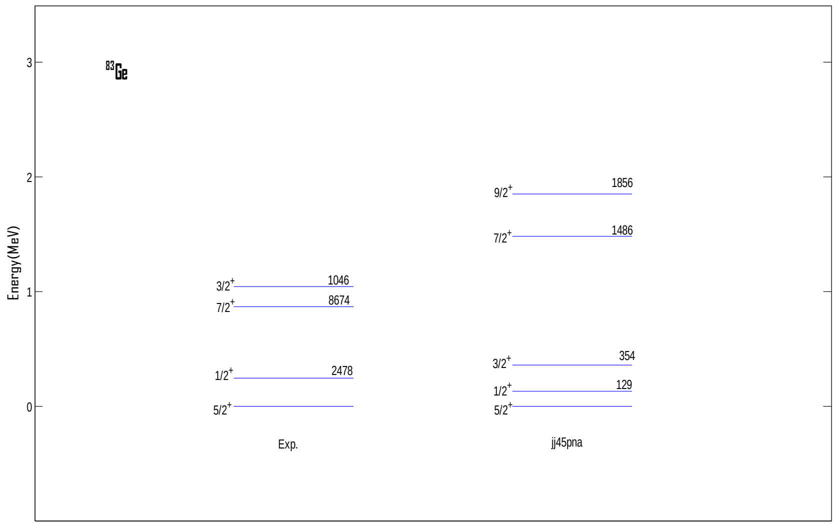

Figure 1. Calculated and experimental spectra for ^{83}Ge.

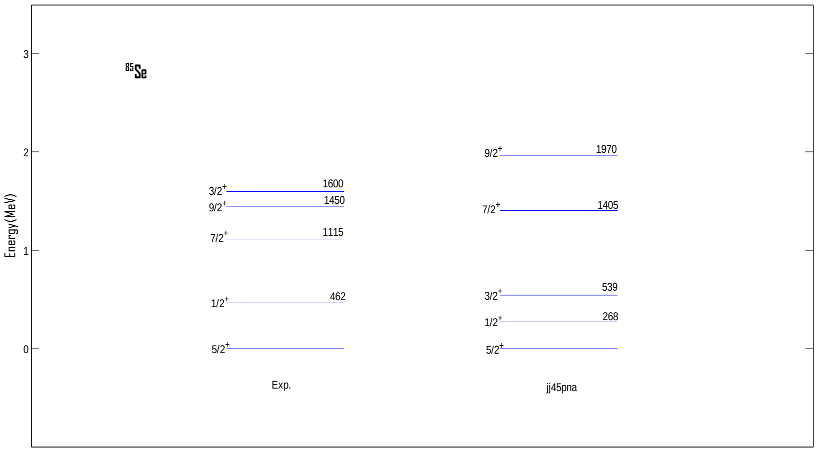

Figure 2. Calculated and experimental spectra for ^{85}Se.

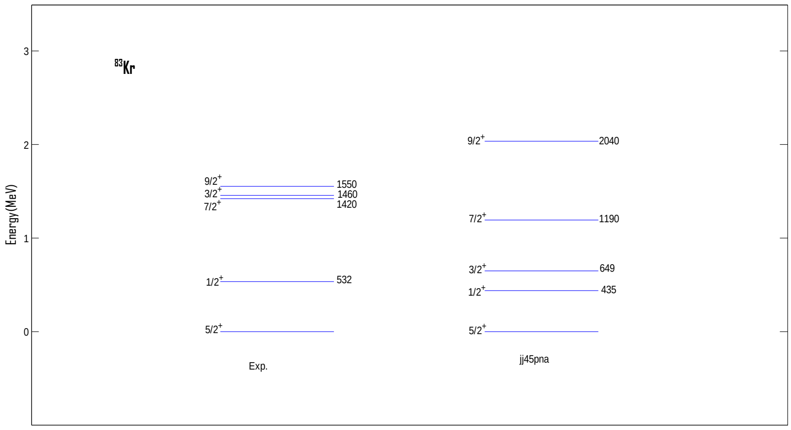

Figure 3. Calculated and experimental spectra for ^{87}Kr.

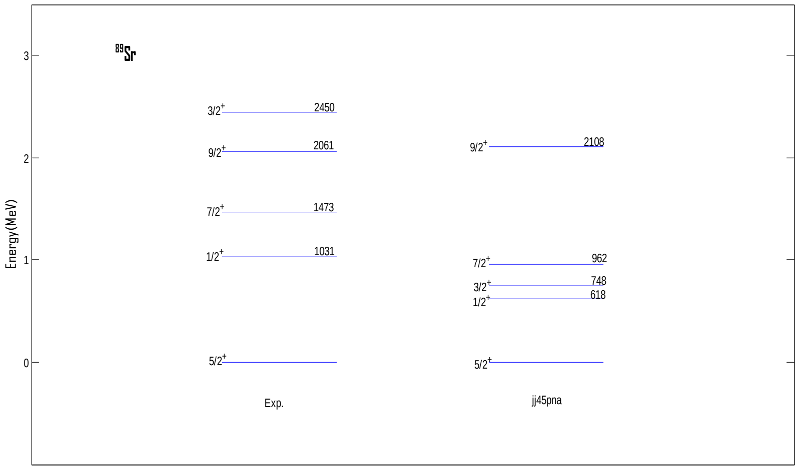

Figure 4. Calculated and experimental spectra for ^{89}Sr.

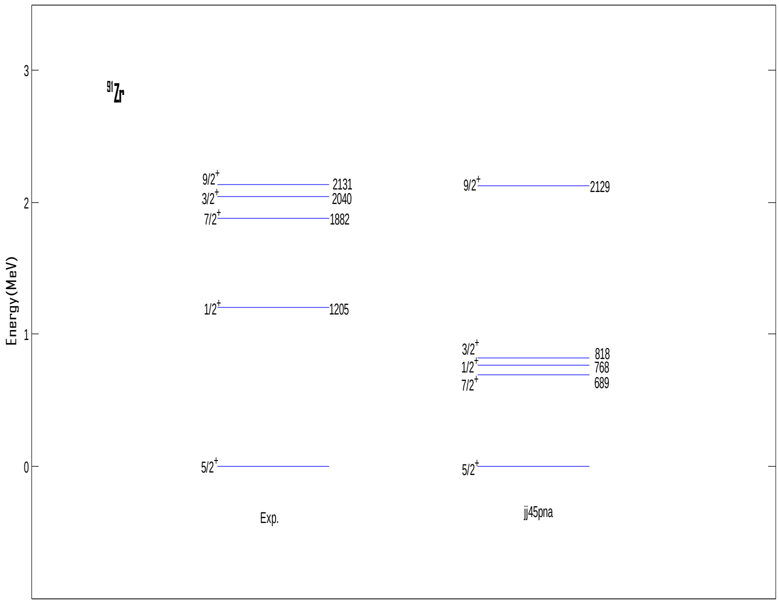

Figure 5. Calculated and experimental spectra for ^{91}Zr.

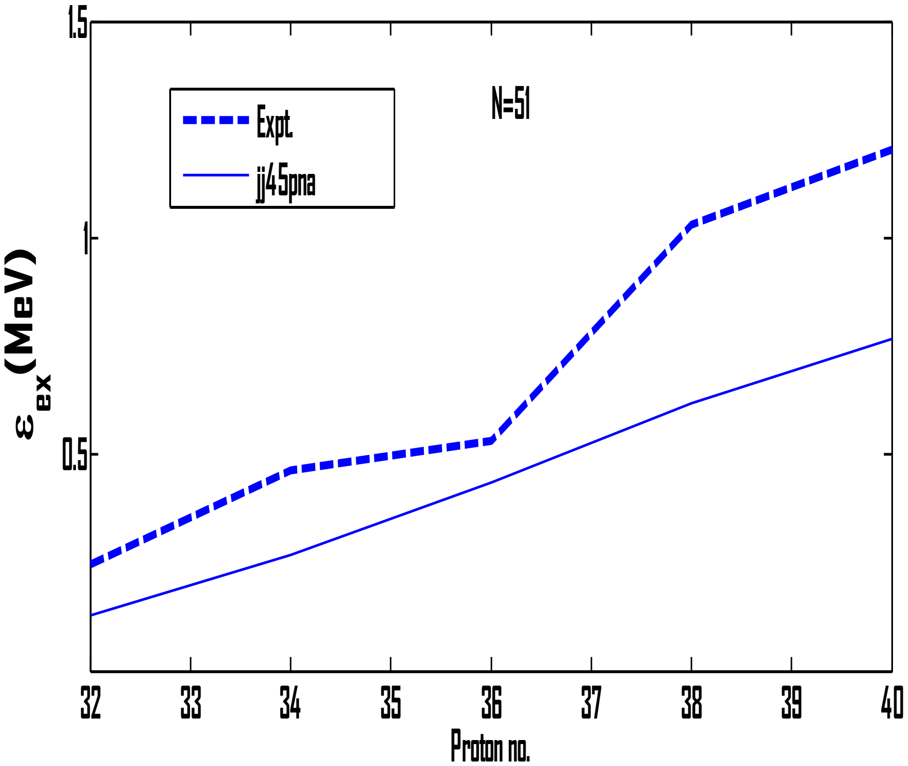

Figure 6. Variation of E(1/2+) with proton no.

Table 1. Main configurations in the wave functions of the ground state and first exited state for $N = 51$ isotones.

Nuclei	J^{π}	Wave function		Probability
		Proton	Neutron	
^{83}Ge	$5/2^+_{gs}$	$(f_{5/2})^2,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^2$	$(d_{5/2})^1$	34.3
	$1/2^+_1$	$(f_{5/2})^2,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^2$	$(s_{1/2})^1$	27.0
	$7/2^+_2$	$(f_{5/2})^2,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^2$	$(g_{7/2})^1$	16.2
	$3/2^+_3$	$(f_{5/2})^2,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^2$	$(d_{3/2})^1$	32.9
^{85}Se	$5/2^+_{gs}$	$(f_{5/2})^4,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^2$	$(d_{5/2})^1$	20.0
	$1/2^+_1$	$(f_{5/2})^4,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^2$	$(s_{1/2})^1$	15.6
	$7/2^+_2$	$(f_{5/2})^2,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^4$	$(g_{7/2})^1$	17.0
	$3/2^+_3$	$(f_{5/2})^4,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^2$	$(d_{3/2})^1$	19.9
^{87}Kr	$5/2^+_{gs}$	$(f_{5/2})^4,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^4$	$(d_{5/2})^1$	19.0
	$1/2^+_1$	$(f_{5/2})^4,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^4$	$(s_{1/2})^1$	14.4
	$7/2^+_2$	$(f_{5/2})^4,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^4$	$(g_{7/2})^1$	22.4
	$3/2^+_3$	$(f_{5/2})^4,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^4$	$(d_{3/2})^1$	19.5
^{89}Sr	$5/2^+_{gs}$	$(f_{5/2})^4,(p_{3/2})^2,(p_{1/2})^0,(g_{9/2})^4$	$(d_{5/2})^1$	14.7
	$1/2^+_1$	$(f_{5/2})^4,(p_{3/2})^2,(p_{1/2})^0,(g_{9/2})^4$	$(s_{1/2})^1$	11.8
	$7/2^+_2$	$(f_{5/2})^4,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^6$	$(g_{7/2})^1$	16.5
	$3/2^+_3$	$(f_{5/2})^4,(p_{3/2})^2,(p_{1/2})^0,(g_{9/2})^4$	$(d_{3/2})^1$	14.1
^{91}Zr	$5/2^+_{gs}$	$(f_{5/2})^6,(p_{3/2})^2,(p_{1/2})^0,(g_{9/2})^4$	$(d_{5/2})^1$	12.4
	$1/2^+_1$	$(f_{5/2})^4,(p_{3/2})^2,(p_{1/2})^0,(g_{9/2})^6$	$(s_{1/2})^1$	9.1
	$7/2^+_2$	$(f_{5/2})^6,(p_{3/2})^0,(p_{1/2})^0,(g_{9/2})^6$	$(g_{7/2})^1$	14.3
	$3/2^+_3$	$(f_{5/2})^4,(p_{3/2})^2,(p_{1/2})^0,(g_{9/2})^6$	$(d_{3/2})^1$	11.3

Table 2. The $B(E2)$ values for $N = 51$ isotones calculated with $e_{\pi}^{eff} = 1.50e$ and $e_{\nu}^{eff} = 0.5e$.

-	^{83}Ge	^{85}Se	^{87}Kr	^{89}Sr
B(E2; $1/2^+ \rightarrow 5/2^+$)(W.u.)	17.9	24.5	26.7	12.7
B(E2; $7/2^+ \rightarrow 5/2^+$)(W.u.)	32.0	17.2	11.2	0.9

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