Proton single-particle energy gaps in Sc isotopes

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Abstract. Variation in the proton single-particle energy gaps is investigated within the framework of nuclear shell model. The change is identified to originate mainly from the central force of the proton-neutron interaction. The relationship between the nuclear state and the single-particle energy gap is discussed. The first 3/2+ state of 53Sc reveals the fragile character of N = 34 semi-magic shell gap.

1 Introduction

Since the beginning of the twenty-first century, the physics of the neutron-rich nuclei has gained a lot of interest. Shell evolution is one of the intriguing phenomena observed in the neutron-rich nuclei. It reveals that the shell structure in nuclei changes depending on the N/Z ratio [1, 2]. Following are some examples of the shell evolution: a) the canonical N = 20 and 28 magic shell gaps disappear for Z = 8–12 nuclei [3–9] and Z < 16 nuclei [10, 11], respectively, b) the new semi-magic shell gaps emerge at N = 14, 16 in oxygen [12, 13], and at N = 32 and 34 in calcium [14, 15].

To uncover the origin of shell evolution, many efforts have been made by theoretical nuclear physicists in the past. In the nuclear shell model framework, Otsuka and his collaborators have unveiled that the bare π + ρ meson exchange tensor force

\[ V(1, 2) = f(r)[Y^2.(\sigma_1 \otimes \sigma_2)^2]^0 \] (1)

is a predominant source of the shell evolution [16]. The robust effects of the tensor force on the single-particle energy gaps has been demonstrated in Refs. [16, 17].

As phenomenological nucleon-nucleon interactions are used in the nuclear shell model, a more rigorous method was put forward by Umeya et al., [18] and Smirnova et al., [19, 20] to elucidate the origin of the shell evolution. This method relies on the spin-tensor decomposition [21, 22] that allows to decompose a shell model interaction into its central, spin-orbit and tensor force components and peruse their role in the shell evolution. It has been demonstrated by Umeya et al., [18] that the proton-neutron central force is crucial for the evolution of the N = 8 shell gap. On the other hand, it has been shown by Smirnova et al., [19] that both proton-neutron central and tensor forces are important for the evolution of N = 20 and 28 shell gaps.

In this article, we intend to discuss the effects of proton-neutron force and its different components on the proton single-particle energy gaps in Sc isotopes. Recently, the low-energy states of neutron-rich 53,55Sc has been populated in the experiments [23, 24]. Among the observed states, their first 3/2+ state have been found near 2.1 MeV and 0.7 MeV, respectively. As such these isotopes have N = 32 and 34 semi-magic shell gaps in their neutron space, so, if the excitation energy of their 3/2+ state is compared with that of 49Sc which is about 3.1 MeV, it can be put forward that the proton 1p3/2 − 0f1/2 magic shell gap present at N = 28 reduces at N = 32 and 34, in particular, substantially at the latter. With motivation to obtain comprehensive information about this point, we have carried out the theoretical investigation within the framework of nuclear shell model. The calculations were performed in the pf harmonic oscillator shell using the GX1N interaction [25]. Here we discuss the results of those calculations.

This article is organized as follows. In Sec. 2, we have given a brief introduction of the effective single-particle energy and the spin-tensor decomposition. In Sec. 3.1, we have discussed the effects of the proton-neutron interaction and its different components on proton-single particle energy gaps. In Sec. 3.2, we have perused the relationship between the 1p3/2 − 0f1/2 proton single-particle energy gap and the first 3/2+ state of 49,53,55Sc. The summary of this work is presented in Sec. 4.

2 Effective single particle energy and spin-tensor decomposition

In the nuclear shell model, the effective single particle energy ESPE gauges the shift in the single-particle energy of an orbit j caused by valence nucleons. The ESPE is determined from the monopole component of shell model Hamiltonian \[ \hat{H} \]. In proton-neutron formalism,
the monopole Hamiltonian $\hat{H}_m$ is expressed as [26, 27]

$$\hat{H}_m = \sum_i \epsilon_i \hat{n}_i + \sum_i \epsilon_i \hat{\rho}_i + \sum_{i<j} \hat{\rho}_i (\hat{n}_j - \delta_{ij}) \hat{\rho}_j = \frac{1}{1 + \delta_{ij}} \hat{\rho}_i \hat{\rho}_j$$

where, $\hat{\rho}_i$ is number operator for particle type $\rho$ and orbit $i$. The index $i$ consists of all quantum numbers $(n, l, \ell)$ to define the orbit, and $\epsilon$ is the unperturbed single-particle energy of that orbit. $\hat{V}$ is total angular momentum $(J)$ averaged NN matrix elements

$$\hat{V}^{\rho \rho'}_{ij} = \sum_{\nu=1}^{\infty} \frac{\epsilon_i (2J+1) (1+(-1)^j \delta_{\rho\rho'} \delta_{ij}) \hat{V}^{\rho \rho'}_{ij}}{(2l+1)(2j+1) - \delta_{\rho\rho'} \delta_{ij}},$$

where, summation runs only over the Pauli principle allowed $J$ values.

In a simple approximation, the $ESPE$ of orbit $j$ for particle $\rho$ can be obtained from the differentiation of the monopole Hamiltonian with respect to particle number $n$ [28]

$$\epsilon_j^{\rho} \equiv \frac{\partial \langle \hat{H}_m \rangle}{\partial n_j} \approx \epsilon_j^{\rho} + \sum_{\rho'} n_{\rho'} \hat{V}^{\rho \rho'}_{jj}.$$ (4)

For the proton orbit $j$ in Sc isotopes, the above expression of $ESPE$ can be rewritten as

$$\epsilon_j^{p} = \epsilon_j^p + \sum_{\rho'} n_{\rho'} \hat{V}^{p \rho'}_{jj}.$$ (5)

Here, the sum runs over the neutron orbit.

At any time, the information about the single-particle energy gaps can be obtained from the effective single-particle energy of the orbits. The spin-tensor decomposition [21, 22] has remained a handy method to gain knowledge about the different forces of an effective interaction. Since nucleons are spin 1/2 fermions, the interaction between two nucleons can be written as the linear sum of the scalar product of configuration space operator $Q$ and spin space operator $S$

$$V = \sum_{k=0}^{2} V(k) = \sum_{k=0}^{2} Q^k S^k.$$

where, rank $k = 0, 1$ and 2 represent central, spin-orbit and tensor force, respectively. To obtain the matrix elements of these force in $jj$ coupling, one needs to transform the $jj$ coupled state into to $LS$ coupled state in the standard way. In the $LS$ coupled state, the matrix of $V(k)$ can be obtained from $V$ as

$$\langle (ab), LS; JM|V(k)|(cd), LS'; JM \rangle = (2k+1)(-1)^l \times \left\{ \begin{array}{ccc} L & S & J \\ S' & L' & k \end{array} \right\} \sum_{J'} (-1)^{J'} (2J'+1) \left\{ \begin{array}{ccc} L & S & J' \\ S' & L' & k \end{array} \right\} \times \langle (ab), LS; J'M|V(k)|(cd), LS'; J'M \rangle,$$

where, $a$ is shorthand notation for the quantum numbers $n_a$ and $l_a$. We have followed this method to obtain the central spin-orbit and tensor force matrix elements of GX1N interaction.

3 Results and discussion

3.1 Proton single-particle energy gaps

Figure 1 presents the single particle energy of proton $pf$ orbits in Sc isotopes. Although these orbits evolve more or less similarly, they build unique patterns for the proton single-particle energy gaps. When neutrons occupy $0f_{7/2}$ and $0f_{5/2}$ orbits, the $1p_{3/2} - 0f_{7/2}$ and $1p_{1/2} - 0f_{5/2}$ proton energy gaps enhance. However, when neutrons occupy $1p_{1/2}$ and $1p_{3/2}$ orbits, the same single-particle energy gaps reduce. Particularly, the $\pi 1p_{3/2} - \pi 0f_{7/2}$ energy gap reduces so much at $N = 34$ relative to $N = 28$, which in a way supports the low excitation energy of $3/2^-$ state of $^{52}$Sc. There is an interesting pattern in the $0f_{7/2} - 0f_{5/2}$ energy gap. Unlike the others two gaps, this energy gap remain approximately constant, which manifest that the splitting of spin-orbit partners are independent from the condition that which orbit is occupied by neutrons.

In Fig. 2, we show the effects of the central, spin-orbit, and tensor forces components of the proton-neutron force on the proton single-particle gaps. It can be easily followed that when neutrons occupy $0f_{7/2}$ and $0f_{5/2}$ orbits, the central force predominantly contributes to enhance the $1p_{3/2} - 0f_{7/2}$ and $1p_{1/2} - 0f_{5/2}$ energy gaps. The same is observed when neutrons occupy $1p_{3/2}$ and $1p_{1/2}$ orbits, however, this time central force acts with the opposite effect, which cause narrowing of gaps. It is worth mentioning here that tensor force tries to widen the $1p_{1/2} - 0f_{7/2}$ energy gap when the $1p_{1/2}$ orbit is filled with neutrons. But, its effect is negated by the central force which contributes with nearly twice of its strength. Further, it can be observed that the central force enhances the $1p_{3/2} - 0f_{7/2}$ and $1p_{1/2} - 0f_{5/2}$ energy gaps by about 0.5 MeV irrespective of $j$ of neutron $0f$ orbits, and similarly reduce the same.
Above we have seen that the 1 \( p_{3/2} \) - 0 \( f_{7/2} \) proton gap reduces from \( N = 28 \) to \( N = 34 \), however, this is not compulsory that its effect will directly appear in the excited states [30], because the single-particle energy gaps are calculated using simple configurations of nucleons. To correlate the 1 \( p_{3/2} \) - 0 \( f_{7/2} \) proton gap with the first 3/2\(^{-}\) state of \(^{49,53,55}\)Sc, we first need to take into account the effects of other configurations. Thus, we have performed full space shell model calculation using the shell model code NuShellX [31]. We have calculated the excitation energy of the 3/2\(^{-}\) state and also the proton transfer spectroscopic factor \( C^2\)S for the ground state 7/2\(^{-}\) and the 3/2\(^{-}\) state. These spectroscopic factors are determined with respect to \(^{1-1}\)Ca isotopes, which signifies how likely it is for the transferred proton to occupy 0 \( f_{7/2} \) and 1 \( p_{3/2} \) proton orbits for the 7/2\(^{-}\) and 3/2\(^{-}\) states, respectively. The theoretical results are given in Fig. 3 along with experimental data [23, 24, 32]. It can be seen that theory nicely reproduce the experimental data.

![Figure 2](https://example.com/figure2.png)

**Figure 2.** Contribution of proton-neutron central, spin-orbit and tensor force in the proton-single particle energy gaps. The gaps are represented as the difference of two matrix elements \( \bar{V}^{\pi}_{n_{j1}} - \bar{V}^{\pi}_{n_{j1}} \) at a time.

![Figure 3](https://example.com/figure3.png)

**Figure 3.** Upper part: The excitation energy of the first 3/2\(^{-}\) state of \(^{49,53,55}\)Sc. Lower part: proton transfer spectroscopic factor for the ground state and the first 3/2\(^{-}\) state of \(^{49,53,55}\)Sc.

As can be observed for \(^{49,53}\)Sc that the proton single-particle strength is about 90 percent in the ground state, and about 40 percent in the 3/2\(^{-}\) state, which is a splendid value for excited states. Thus, the drop of the excitation energy of the 3/2\(^{-}\) state from \(^{49}\)Sc to \(^{55}\)Sc can be attributed to the narrowing of 1 \( p_{3/2} \) - 0 \( f_{7/2} \) single-particle energy gap. In the 3/2\(^{-}\) state of \(^{55}\)Sc, the single-particle strength is small, so, the further drop of the excitation energy cannot be accounted to 1 \( p_{3/2} \) - 0 \( f_{7/2} \) energy gap. The occupation numbers of neutron 1 \( p_{1/2} \) and 0 \( f_{5/2} \) orbits for this state are 1.06, and 1.07, respectively, which infer that it originates from the transition of a neutron across \( N = 34 \) semi-magic shell gap. However, as its excitation energy is small, this
manifests that \( N = 34 \) semi-magic shell gap is fragile by nature. The third \( 3/2^- \) state of \(^{55}\text{Sc}\) is found to own about 40 percent of total proton single-particle strength, but, it lies at 2.5 MeV. The high excitation energy of this state seems to be endowed by the higher order correlations.

4 Summary

In this work, we investigated the effects of proton-neutron force and its different components on the proton single-particle energy gaps. The calculations were performed for Sc isotopes within the nuclear shell model framework. It was found that the \( 0f_{5/2}^f-0f_{7/2}^f \) energy gap remains nearly constant, while, \( 1p_{3/2}^p-0f_{7/2}^f \) and \( 1p_{1/2}^p-0f_{7/2}^f \) energy gaps enhance and reduce depending on the orbit occupied by neutrons. Mainly the central force was identified causing these changes in the gaps. Further, it was observed that the drop of the excitation energy of the first \( 3/2^- \) from \(^{49}\text{Sc}\) to \(^{53}\text{Sc}\) is due to the shrink of \( 1p_{3/2}^p-0f_{7/2}^f \) gap. However, the subsequent drop of the excitation energy at \(^{55}\text{Sc}\) is not associated with this gap. The \( 3/2^- \) state of \(^{55}\text{Sc}\) gain its energy particularly from the transition of neutron across \( N = 34 \) semi-magic shell gap, but since the excitation energy is low, this exhibits that the \( N = 34 \) semi-magic shell gap is fragile by nature.

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References